

Ab Initio Calculation of Vibrational Absorption and Circ Density Functional Force Fields

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| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 217 | Experimentelle und quantenchemische Untersuchungen zum Schwingungsspektrum des Dimethyltrithiocarbonats. Zeitschrift Fur Physikalische Chemie, 1995, 191, 159-177. | 1.4 | 5 |
| 218 | Eine ungewöhnliche intermolekulare Dreizentren-H ₂ Re-Wasserstoffbrücke zwischen [ReH ₅ (PPh ₃) ₃] und Indol im Kristall. Angewandte Chemie, 1995, 107, 2711-2713. | 1.6 | 22 |
| 219 | An Unconventional Intermolecular Three-Center N-H ₂ Re Hydrogen Bond in Crystalline [ReH ₅ (PPh ₃) ₃]·indole·C ₆ H ₆ . Angewandte Chemie International Edition in English, 1995, 34, 2507-2509. | 4.4 | 195 |
| 220 | On the interaction of CO and NH ₃ with BH ₃ and BF ₃ . Chemical Physics Letters, 1995, 237, 14-19. | 1.2 | 44 |
| 221 | The bond dissociation energies of 1-butene. Chemical Physics Letters, 1995, 239, 252-257. | 1.2 | 14 |
| 222 | What is the structure of FeC ₅ H ₆ ?. Chemical Physics Letters, 1995, 240, 526-532. | 1.2 | 9 |
| 223 | The MCH ₂ ⁺ systems: do ScCH ₂ ⁺ and TiCH ₂ ⁺ have Cs or C _{2v} symmetry and a comparison of the B3LYP method to other approaches. Chemical Physics Letters, 1995, 245, 150-157. | 1.2 | 60 |
| 224 | A comparison of correlation-consistent and Pople-type basis sets. Chemical Physics Letters, 1995, 245, 158-164. | 1.2 | 5 |
| 225 | The dissociation energies of AlH ₂ and AlAr. Chemical Physics Letters, 1995, 246, 33-39. | 1.2 | 29 |
| 226 | A comparison of the accuracy of different functionals. Chemical Physics Letters, 1995, 246, 40-44. | 1.2 | 393 |
| 227 | The sensitivity of B3LYP atomization energies to the basis set and a comparison of basis set requirements for CCSD(T) and B3LYP. Chemical Physics Letters, 1995, 240, 533-540. | 1.2 | 272 |
| 228 | Density functional theory calculations of molecular structures and harmonic vibrational frequencies using hybrid density functionals. Computational and Theoretical Chemistry, 1995, 357, 225-235. | 1.5 | 126 |
| 229 | Thermochemistry of disulfur decafluoride, S ₂ F ₁₀ . Journal of Chemical Physics, 1995, 103, 10162-10168. | 1.2 | 5 |
| 230 | A modification of the Gaussian-2 approach using density functional theory. Journal of Chemical Physics, 1995, 103, 1788-1791. | 1.2 | 424 |
| 231 | Barriers for hydrogen atom diffusion on the Si(100)-1 surface. Journal of Chemical Physics, 1995, 102, 8249-8254. | 1.2 | 45 |
| 232 | NADEL SHEAVES AND PROPERTIES OF VECTOR BUNDLES ON FANO VARIETIES. Izvestiya Mathematics, 1995, 45, 281-295. | 0.1 | 0 |
| 233 | The dissociation energies of CH ₄ and C ₂ H ₂ revisited. Journal of Chemical Physics, 1995, 103, 10589-10596. | 1.2 | 38 |
| 234 | Basis set convergence and performance of density functional theory including exact exchange contributions for geometries and harmonic frequencies. Molecular Physics, 1995, 86, 1437-1450. | 0.8 | 164 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 236 | A Reassessment of the Bond Dissociation Energies of Peroxides. <i>Ab Initio Study</i> . Journal of the American Chemical Society, 1996, 118, 12758-12765. | 6.6 | 262 |
| 237 | A comparison of models for calculating nuclear magnetic resonance shielding tensors. Journal of Chemical Physics, 1996, 104, 5497-5509. | 1.2 | 2,106 |
| 238 | Reactions of Laser-Ablated Iron Atoms with Oxygen Molecules in Condensing Argon. Infrared Spectra and Density Functional Calculations of Iron Oxide Product Molecules. The Journal of Physical Chemistry, 1996, 100, 5261-5273. | 2.9 | 152 |
| 239 | Basis Set and Correlation Effects on Transition State Geometries and Kinetic Isotope Effects. The Journal of Physical Chemistry, 1996, 100, 16892-16898. | 2.9 | 18 |
| 240 | Prediction of Vibrational Circular Dichroism Spectra Using Density Functional Theory: Δ -Camphor and Fenchone. Journal of the American Chemical Society, 1996, 118, 6327-6328. | 6.6 | 80 |
| 241 | Theoretical Infrared Spectra for Polycyclic Aromatic Hydrocarbon Neutrals, Cations, and Anions. The Journal of Physical Chemistry, 1996, 100, 2819-2841. | 2.9 | 433 |
| 242 | Comparison of <i>ab Initio</i> and Density Functional Theory for Alkali Peroxynitrite: A Highly Correlated System with Hartree-Fock Instability. The Journal of Physical Chemistry, 1996, 100, 6942-6949. | 2.9 | 21 |
| 243 | Systematic Model Chemistries Based on Density Functional Theory: Comparison with traditional Models and with Experiment. Theoretical and Computational Chemistry, 1996, 4, 679-707. | 0.2 | 39 |
| 244 | Density-Functional-Derived Structures, Spin Properties, and Vibrations for Phenol Radical Cation. The Journal of Physical Chemistry, 1996, 100, 10554-10563. | 2.9 | 50 |
| 245 | How Does Fe ⁺ Activate C-C and C-H Bonds in Ethane? A Theoretical Investigation Using Density Functional Theory. The Journal of Physical Chemistry, 1996, 100, 6236-6242. | 2.9 | 163 |
| 246 | Electron Densities of Homonuclear Diatomic Molecules As Calculated from Density Functional Theory. The Journal of Physical Chemistry, 1996, 100, 5274-5280. | 2.9 | 20 |
| 247 | Comparative Study of Ethane and Propane Cation Radicals by B3LYP Density Functional and High-Level <i>ab Initio</i> Methods. The Journal of Physical Chemistry, 1996, 100, 15774-15784. | 2.9 | 57 |
| 248 | Origin of the Acidity of Enols and Carboxylic Acids. Journal of the American Chemical Society, 1996, 118, 8291-8299. | 6.6 | 58 |
| 249 | Reactions of Laser-Ablated Iron Atoms with Oxygen Molecules: Matrix Infrared Spectra and Density Functional Calculations of OFeO, FeOO, and Fe(O ₂). Journal of the American Chemical Society, 1996, 118, 467-470. | 6.6 | 101 |
| 250 | Protonated <i>p</i> -Benzoquinone. Journal of Organic Chemistry, 1996, 61, 3167-3171. | 1.7 | 7 |
| 251 | Properties of Closed-Shell, Octahedral, Multiply-Charged Hexafluorometallates MF ₆ ³⁻ , M = Sc, Y, La, ZrF ₆ ²⁻ , and TaF ₆ ⁻ . Journal of the American Chemical Society, 1996, 118, 1173-1180. | 6.6 | 59 |
| 252 | Nature of the Si(SiMe ₃) ₃ ⁺ Cation in Aromatic Solvents. Organometallics, 1996, 15, 5495-5501. | 1.1 | 29 |
| 253 | Infrared Spectroscopic Characterization of Cyanocuprates. Journal of the American Chemical Society, 1996, 118, 8808-8816. | 6.6 | 49 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 254 | Structure of Lithium Bis(diphenylphosphino)amide: An X-ray, NMR, and Modeled Theoretical Study. <i>Organometallics</i> , 1996, 15, 4776-4782. | 1.1 | 31 |
| 255 | Dimeric [3,3-Dimethyl-2-(trimethylsilyl)cyclopropenyl]-lithium-Tetramethylethylenediamine: Distortion of the Cyclopropenyl Geometry Due to Strong Rehybridization at the Lithiated Carbon. <i>Journal of the American Chemical Society</i> , 1996, 118, 1086-1091. | 6.6 | 24 |
| 256 | The C ₇ H ₆ Potential Energy Surface Revisited: Relative Energies and IR Assignment. <i>Journal of the American Chemical Society</i> , 1996, 118, 1535-1542. | 6.6 | 155 |
| 257 | Intramolecularly Stabilized Phenylsilyl and Anthrylsilyl Cations. <i>Organometallics</i> , 1996, 15, 5309-5320. | 1.1 | 42 |
| 258 | Toward Planar Tetracoordinate Carbon in the Puckered Ladder Structures of Chelated Cyclopropenyllithium Aggregates. <i>Journal of the American Chemical Society</i> , 1996, 118, 6924-6933. | 6.6 | 44 |
| 259 | A Theoretical View on Co ⁺ -Mediated C-C and C-H Bond Activations in Ethane. <i>Journal of the American Chemical Society</i> , 1996, 118, 9932-9940. | 6.6 | 104 |
| 260 | Difluorodioxirane: An Unusual Cyclic Peroxide. <i>Journal of the American Chemical Society</i> , 1996, 118, 10595-10608. | 6.6 | 56 |
| 261 | Gas-Phase Bond Strength and Atomic Connectivity Studies of the Unsymmetrical Two-Center Three-Electron Ion, [Et ₂ S ⁺ ~SMe ₂] ⁺ . <i>Journal of the American Chemical Society</i> , 1996, 118, 7836-7842. | 6.6 | 34 |
| 262 | Vibrational Optical Activity. <i>Applied Spectroscopy</i> , 1996, 50, 14A-26A. | 1.2 | 96 |
| 263 | Ab initio calculation of atomic axial tensors and vibrational rotational strengths using density functional theory. <i>Molecular Physics</i> , 1996, 89, 579-594. | 0.8 | 72 |
| 264 | Comparison between Optimized Geometries and Vibrational Frequencies Calculated by the DFT Methods. <i>The Journal of Physical Chemistry</i> , 1996, 100, 15056-15063. | 2.9 | 198 |
| 265 | Observation of the Hammick Intermediate: Reduction of the Pyridine-2-ylid Ion in the Gas Phase. <i>Journal of the American Chemical Society</i> , 1996, 118, 11898-11904. | 6.6 | 84 |
| 266 | Structural and vibrational analysis of indole by density functional and hybrid Hartree-Fock/density functional methods. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1996, , 2653-2662. | 0.9 | 32 |
| 267 | Tautomerism, Ionization, and Bond Dissociations of 5-Nitro-2,4-dihydro-3H-1,2,4-triazolone. <i>Journal of the American Chemical Society</i> , 1996, 118, 8048-8055. | 6.6 | 63 |
| 268 | A theoretical study of the valence and dipole bound states of the nitromethane anion. <i>Journal of Chemical Physics</i> , 1996, 105, 8785-8792. | 1.2 | 120 |
| 269 | The varying nature of fluorine oxygen bonds. <i>Molecular Physics</i> , 1996, 89, 1359-1372. | 0.8 | 6 |
| 270 | Thermochemical Assessment of the Aromatic and Antiaromatic Characters of the Cyclopropenyl Cation, Cyclopropenyl Anion, and Cyclopropenyl Radical: A High-Level Computational Study. <i>The Journal of Physical Chemistry</i> , 1996, 100, 17801-17806. | 2.9 | 64 |
| 271 | Theoretical study of the thio-Claisen rearrangement. Can vinylthioethanimine undergo a [3,3]-sigmatropic shift?. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1996, , 2065-2071. | 0.9 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 272 | Structural and vibrational analysis of indolyl radical and indolyl radical cation from density functional methods. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1996, , 2663. | 0.9 | 25 |
| 273 | Mechanisms of Competitive Ring-Directed and Side-Chain-Directed Metalations in Ortho-Substituted Toluenes. <i>Organometallics</i> , 1996, 15, 3345-3359. | 1.1 | 27 |
| 274 | Charge density in crystalline citrinin from X-ray diffraction at 19â€K. <i>Canadian Journal of Chemistry</i> , 1996, 74, 1145-1161. | 0.6 | 82 |
| 275 | The role of hydrogens in stabilizing organic ions. <i>Canadian Journal of Chemistry</i> , 1996, 74, 892-900. | 0.6 | 32 |
| 276 | Harmonic Vibrational Frequencies:Â An Evaluation of HartreeâˆFock, MÃllerâˆPlesset, Quadratic Configuration Interaction, Density Functional Theory, and Semiempirical Scale Factors. <i>The Journal of Physical Chemistry</i> , 1996, 100, 16502-16513. | 2.9 | 6,586 |
| 277 | Calculation of Ionization Potentials and CâˆH Bond Dissociation Energies of Toluene Derivatives. <i>The Journal of Physical Chemistry</i> , 1996, 100, 2950-2956. | 2.9 | 60 |
| 278 | Performance of pure and hybrid DFT methods in calculations of ethylene iodonium and methyl iodide. <i>Computational and Theoretical Chemistry</i> , 1996, 365, 111-117. | 1.5 | 1 |
| 279 | Vibrational analysis of the spectra of 1,3,4-oxadiazole, 1,3,4-thiadiazole, 1,2,5-oxadiazole and 1,2,5-thiadiazole: comparison between DFT, MP2 and HF force fields. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1996, 52, 33-44. | 2.0 | 38 |
| 280 | Theoretical and experimental studies of F3SiCO+ and F3SiOC+. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1996, 153, 161-172. | 1.9 | 7 |
| 281 | The dissociation energies of FeF, FeCl, and FeBr and their positive ions. <i>Chemical Physics</i> , 1996, 211, 163-169. | 0.9 | 32 |
| 282 | On the photoelectron spectrum of Li4âˆ. <i>Chemical Physics Letters</i> , 1996, 260, 309-313. | 1.2 | 3 |
| 283 | The structure of the methanol radical cation: an artificially short C-O bond with MP2 theory. <i>Chemical Physics Letters</i> , 1996, 262, 187-193. | 1.2 | 22 |
| 284 | Mechanistic Details of the Fe+-Mediated C?C and C?H Bond Activations in Propane: A Theoretical Investigation. <i>Helvetica Chimica Acta</i> , 1996, 79, 1939-1956. | 1.0 | 49 |
| 285 | Theoretische Untersuchungen schlieÃŸen eine [2 + 2]â€Addition als einleitenden Schritt der Osmiumtetroxidâ€katalysierten Dihydroxylierung von Alkenen aus. <i>Angewandte Chemie</i> , 1996, 108, 3008-3011. | 1.6 | 40 |
| 286 | Theoretical study of intramolecular hydrogen bonding and molecular geometry of 2-trifluoromethylphenol. <i>Journal of Computational Chemistry</i> , 1996, 17, 1804-1819. | 1.5 | 24 |
| 287 | Reaction of boron atoms with ethylene: ab initio study of the borirane radical. <i>Chemical Physics Letters</i> , 1996, 250, 421-427. | 1.2 | 14 |
| 288 | Application of density functional theory /Hartree-Fock hybrid methods. Geometries and bond dissociation energies of Al+ complexes. <i>Chemical Physics Letters</i> , 1996, 250, 387-392. | 1.2 | 44 |
| 289 | Formation of OH radicals in the gas phase ozonolysis of alkenes: the unexpected role of carbonyl oxides. <i>Chemical Physics Letters</i> , 1996, 252, 221-229. | 1.2 | 169 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 290 | Ab initio calculation of atomic axial tensors and vibrational rotational strengths using density functional theory. <i>Chemical Physics Letters</i> , 1996, 252, 211-220. | 1.2 | 427 |
| 291 | Optimized molecular integration schemes for density functional theory ab initio molecular dynamics simulations. <i>Chemical Physics Letters</i> , 1996, 255, 187-194. | 1.2 | 17 |
| 292 | Vibrational frequency prediction using density functional theory. <i>Chemical Physics Letters</i> , 1996, 256, 391-399. | 1.2 | 1,141 |
| 293 | Dimesitylketone O-oxide: verification of an unusually stable carbonyl oxide by NMR chemical shift calculations. <i>Chemical Physics Letters</i> , 1996, 260, 43-50. | 1.2 | 24 |
| 294 | The performance of B3-LYP density functional theory in describing SN2 reactions at saturated carbon. <i>Chemical Physics Letters</i> , 1996, 260, 558-564. | 1.2 | 118 |
| 295 | The B(H ₂) ⁿ -H ₂ binding energies, for n = 0-3. <i>Chemical Physics Letters</i> , 1996, 261, 637-643. | 1.2 | 1 |
| 296 | Opening and Closure of the Fullerene Cage in <i>cis</i> -Bisimino Adducts of C ₆₀ : The Influence of the Addition Pattern and the Addend. <i>Chemistry - A European Journal</i> , 1996, 2, 935-943. | 1.7 | 143 |
| 297 | Theory Rules Out a [2+ 2] Addition of Osmium Tetroxide to Olefins as Initial Step of the Dihydroxylation Reaction. <i>Angewandte Chemie International Edition in English</i> , 1996, 35, 2817-2820. | 4.4 | 123 |
| 298 | The structures and relative energies of formamide (H ₂ NCHO) and radical ions H ₂ NCHO ^{•+} , H ₂ NCOH ^{•+} and H ₃ NCO ^{•+} . <i>Chemical Physics</i> , 1996, 202, 243-252. | 0.9 | 3 |
| 299 | The structure of Li ^{•+} and K ^{•+} . <i>Chemical Physics</i> , 1996, 206, 35-42. | 0.9 | 8 |
| 300 | N-Acetyl-L-alanine N ^{•2} -methylamide: a density functional analysis of the vibrational absorption and vibrational circular dichroism spectra. <i>Chemical Physics</i> , 1996, 208, 81-116. | 0.9 | 129 |
| 301 | The structure and stability of B _n ⁺ clusters. <i>Chemical Physics</i> , 1996, 208, 233-242. | 0.9 | 134 |
| 302 | Ab initio MP2 and DFT calculations of geometry and solution tautomerism of purine and some purine derivatives. <i>Chemical Physics</i> , 1996, 211, 147-161. | 0.9 | 89 |
| 303 | Experimental and theoretical studies of FeC ₇ H ₇ ⁺ isomers: Fe-C ₇ H ₇ bond energies and isomeric differentiation. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1996, 157-158, 249-263. | 1.9 | 10 |
| 304 | Molecular and electronic structure of 1,2-disilacyclobutabenzene. Ab initio molecular orbital and density functional study. <i>Journal of Organometallic Chemistry</i> , 1996, 524, 107-114. | 0.8 | 11 |
| 305 | Theoretical and experimental studies of the structure and vibrational spectra of NTO. <i>Journal of Molecular Structure</i> , 1996, 384, 87-99. | 1.8 | 46 |
| 306 | Radical Cation of 1,3-Butadiene: A Resonance Raman Spectrum of Deuterated Derivatives and Improved Force Field. <i>The Journal of Physical Chemistry</i> , 1996, 100, 16850-16855. | 2.9 | 17 |
| 307 | Electron Densities of Several Small Molecules As Calculated from Density Functional Theory. <i>The Journal of Physical Chemistry</i> , 1996, 100, 6317-6324. | 2.9 | 35 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 308 | An Assessment of Density Functional Methods for Calculating Thermochemistries of Si-H-Cl Compounds. The Journal of Physical Chemistry, 1996, 100, 5-8. | 2.9 | 32 |
| 309 | Density Functional Theory Study of Vibrational Spectra of Fluorene. The Journal of Physical Chemistry, 1996, 100, 8782-8785. | 2.9 | 63 |
| 310 | Vibrational Circular Dichroism. , 1996, , 555-598. | | 60 |
| 311 | Dissociative electron attachment and intramolecular electron transfer in linear haloalkenes. Journal of Chemical Physics, 1996, 105, 7896-7903. | 1.2 | 13 |
| 312 | Computational Study of the Thermochemistry of C5H5+Isomers: Which C5H5+Isomer Is the Most Stable?. The Journal of Physical Chemistry, 1996, 100, 10952-10955. | 2.9 | 42 |
| 313 | Adsorption of water and methanol on zeolite Bronsted acid sites: An ab initio, embedded cluster study including electron correlation. Journal of Chemical Physics, 1996, 105, 3770-3776. | 1.2 | 77 |
| 314 | Investigation of the reliability of density functional methods: Reaction and activation energies for Si-Si bond cleavage and H2 elimination from silanes. Journal of Chemical Physics, 1996, 104, 148-158. | 1.2 | 112 |
| 315 | Microwave spectrum, large amplitude motions, and ab initio calculations for N2O5. Journal of Chemical Physics, 1996, 105, 7249-7262. | 1.2 | 14 |
| 316 | Ab Initio Calculation of Vibrational Absorption and Circular Dichroism Spectra: 6,8-Dioxabicyclo[3.2.1]octane. The Journal of Physical Chemistry, 1996, 100, 9262-9270. | 2.9 | 34 |
| 317 | Density Functional and MP2 Calculations of Spin Densities of Oxidized 3-Methylindole: Models for Tryptophan Radicals. The Journal of Physical Chemistry, 1996, 100, 954-959. | 2.9 | 57 |
| 318 | Thermochemistry of Tetrazete and Tetraazetetrahedrane: A High-Level Computational Study. The Journal of Physical Chemistry, 1996, 100, 1569-1577. | 2.9 | 34 |
| 319 | Infrared Spectra and Quantum Chemical Calculations of Group 2 MO2, O2MO2, and Related Molecules. The Journal of Physical Chemistry, 1996, 100, 10088-10099. | 2.9 | 57 |
| 320 | Fluoroformyl Hypofluorite, Fluoroformyl Peroxyhypofluorite, and Fluoroformyl Peroxide. A Density Functional Study. The Journal of Physical Chemistry, 1996, 100, 11292-11296. | 2.9 | 11 |
| 321 | Visible Light-Induced Reaction of NO2 with Propene in Low-Temperature Argon and Xenon Matrices. The Journal of Physical Chemistry, 1996, 100, 15815-15820. | 2.9 | 14 |
| 322 | Molecular Structures and Vibrational Spectra of Pyrrole and Carbazole by Density Functional Theory and Conventional ab Initio Calculations. The Journal of Physical Chemistry, 1996, 100, 15073-15078. | 2.9 | 111 |
| 323 | Reactions of Selenium in a Quartz Discharge Tube. Infrared Spectra and Density Functional Theory Calculations of New Selenium-Nitrogen and Selenium-Silicon Species in Solid Argon. The Journal of Physical Chemistry, 1996, 100, 16667-16673. | 2.9 | 12 |
| 324 | Density Functional Studies of Vibrational Properties of HCN, H2O, CH2O, CH4, and C2H4. The Journal of Physical Chemistry, 1996, 100, 16530-16537. | 2.9 | 21 |
| 325 | Structural Properties of [(Trichlorosilyl)amino]dichloroborane. The Journal of Physical Chemistry, 1996, 100, 16551-16554. | 2.9 | 11 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 326 | Chemical storage of data. <i>Nanotechnology</i> , 1997, 8, 1-5. | 1.3 | 18 |
| 327 | The structure and stability of BnH ⁺ clusters. <i>Journal of Chemical Physics</i> , 1997, 106, 2317-2322. | 1.2 | 43 |
| 328 | Ab initio molecular dynamics simulation of H ₅ O ₂ ⁺ and H ₇ O ₃ ⁺ gas phase clusters based on density functional theory. <i>Molecular Physics</i> , 1997, 91, 963-975. | 0.8 | 9 |
| 329 | Quantitative Analyses of Cieplak vs. Felkin-Anh Effects in Hydride Reduction of Cyclohexanone. <i>Chemistry Letters</i> , 1997, 26, 431-432. | 0.7 | 10 |
| 330 | Comparative Ab initio and Hybrid DFT Studies Relevant to an Experimental Investigation of Neutral and Cationic [Si, P, H ₂] Isomers. <i>Bulletin of the Chemical Society of Japan</i> , 1997, 70, 777-787. | 2.0 | 8 |
| 331 | Cation-π Interaction in Al(L) ⁺ Complexes (L = C ₆ H ₆ , C ₅ H ₅ N, C ₅ H ₆ , C ₄ H ₄ NH, C ₄ H ₄ O). <i>Journal of Physical Chemistry A</i> , 1997, 101, 3800-3807. | 1.1 | 47 |
| 332 | Inherently Hindered Rotation about a Disulfide Bond. <i>Journal of the American Chemical Society</i> , 1997, 119, 12685-12686. | 6.6 | 25 |
| 333 | Reactions of Laser-Ablated Copper Atoms with Dioxygen. Infrared Spectra of the Copper Oxides CuO, OCuO, CuOCuO, and OCuOCuO and Superoxide CuOO in Solid Argon. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4026-4034. | 1.1 | 74 |
| 334 | Ab Initio Study of the Hydrogen Bonding between Pyrrole and Hydrogen Fluoride: A Comparison of NH⋯F and FH⋯ interactions. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1982-1988. | 1.1 | 27 |
| 335 | Computer simulation of zeolite structure and reactivity using embedded cluster methods. <i>Faraday Discussions</i> , 1997, 106, 79-92. | 1.6 | 190 |
| 336 | A Density Functional Study of 2-Lithio-1,3-dithiane and 2-Lithio-2-phenyl-1,3-dithiane: A Conformational Preference of the C ^δ -Li Bond and Structural Analysis. <i>Journal of the American Chemical Society</i> , 1997, 119, 7545-7549. | 6.6 | 42 |
| 337 | Nature of the Transition Structure for Alkene Epoxidation by Peroxyformic Acid, Dioxirane, and Dimethyldioxirane: A Comparison of B3LYP Density Functional Theory with Higher Computational Levels. <i>Journal of Physical Chemistry A</i> , 1997, 101, 6092-6100. | 1.1 | 102 |
| 338 | On the Reaction of FNO ₂ with CH ₃ , tert-Butyl, and C ₁₃ H ₂₁ . <i>Journal of Physical Chemistry A</i> , 1997, 101, 1188-1192. | 1.1 | 21 |
| 339 | Charge-Localizing Effect in Alkali-Metal Enolates and Phenolates. Structure and Aromaticity of the Phenolate Anion. <i>Organometallics</i> , 1997, 16, 737-746. | 1.1 | 30 |
| 340 | Binding of Nitric Oxide to First-Transition-Row Metal Cations: An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8530-8539. | 1.1 | 71 |
| 341 | Successive OH Binding Energies of M(OH) _n ⁺ for n = 1-3 and M = Sc, Ti, V, Co, Ni, and Cu. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8949-8955. | 1.1 | 53 |
| 342 | Kinetic and Theoretical Investigation of the Gas-Phase Ozonolysis of Isoprene: Carbonyl Oxides as an Important Source for OH Radicals in the Atmosphere. <i>Journal of the American Chemical Society</i> , 1997, 119, 7330-7342. | 6.6 | 168 |
| 343 | Ab Initio Density Functional Computations of Conformations and Bond Dissociation Energies for Hexahydro-1,3,5-trinitro-1,3,5-triazine. <i>Journal of the American Chemical Society</i> , 1997, 119, 6583-6589. | 6.6 | 148 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 344 | Trimethyl-p-benzoquinone Provides Excellent Structural, Spectroscopic, and Thermochemical Models for Plastoquinone-1 and Its Radical Anion. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1160-1165. | 1.1 | 34 |
| 345 | A Comparison of the Properties of Various Fused-Ring Quinones and Their Radical Anions Using Hartree-Fock and Hybrid Hartree-Fock/Density Functional Methods. <i>Journal of Physical Chemistry A</i> , 1997, 101, 7154-7166. | 1.1 | 54 |
| 346 | Ab Initio Prediction of Vibrational Absorption and Circular Dichroism Spectra of Chiral Natural Products Using Density Functional Theory: Δ -Pinene. <i>Journal of Physical Chemistry A</i> , 1997, 101, 9912-9924. | 1.1 | 124 |
| 347 | Theoretical Study of Ion Pair SN2 Reactions: Ethyl vs Methyl Reactivities and Extension to Higher Alkyls. <i>Journal of the American Chemical Society</i> , 1997, 119, 5013-5019. | 6.6 | 66 |
| 348 | Ab Initio Prediction of Vibrational Absorption and Circular Dichroism Spectra of Chiral Natural Products Using Density Functional Theory: Camphor and Fenchone. <i>Journal of Physical Chemistry A</i> , 1997, 101, 6322-6333. | 1.1 | 99 |
| 349 | Reactions of Laser-Ablated Aluminum Atoms with Ammonia. Infrared Spectra of HAlNH_2 , AlNH_2 , and HAlNH in Solid Argon. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5082-5089. | 1.1 | 32 |
| 350 | Structure and Vibrations of the C_2P and CNP Radicals and Their Cations Using Density Functional and Coupled Cluster Theories. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8319-8326. | 1.1 | 19 |
| 351 | Molecular and Vibrational Structure of 1,6,6a-trithiapentalene. Infrared Linear Dichroism Spectroscopy and ab Initio Normal-Mode Analyses. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4475-4480. | 1.1 | 19 |
| 352 | Dimesityldioxirane. <i>Journal of the American Chemical Society</i> , 1997, 119, 7265-7270. | 6.6 | 57 |
| 353 | Theoretical Study of Tungsten Carbonyl Complexes ($n = 1-6$): Structures, Binding Energies, and Implications for Gas Phase Reactivities. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3966-3976. | 1.1 | 19 |
| 354 | The C_4H_4^+ Potential Energy Surface. 2. The Jahn-Teller Stabilization of Ionized Tetrahedrane and Its Rearrangement to Cyclobutadiene Radical Cation. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3918-3924. | 1.1 | 18 |
| 355 | Ab Initio Study of Hydrogen Abstraction Reactions. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4416-4431. | 1.1 | 105 |
| 356 | Photochemistry of p-Benzoquinone Diazide Carboxylic Acids: Formation of 2,4-Didehydrophenols. <i>Journal of the American Chemical Society</i> , 1997, 119, 10660-10672. | 6.6 | 34 |
| 357 | The Tris(9-borabicyclo[3.3.1]nonyl)silylium Cation: A Suggestion for a Weakly Coordinated Silylium Cation in Solution. <i>Organometallics</i> , 1997, 16, 2377-2385. | 1.1 | 16 |
| 358 | Performance of the B3LYP/ECP DFT Calculations of Iron-Containing Compounds. <i>Journal of Physical Chemistry A</i> , 1997, 101, 316-323. | 1.1 | 123 |
| 359 | Infrared Spectra of Perdeuterated Naphthalene, Phenanthrene, Chrysene, and Pyrene. <i>Journal of Physical Chemistry A</i> , 1997, 101, 2414-2422. | 1.1 | 61 |
| 360 | Structure and Bonding of the Isoelectronic Hexacarbonyls $[\text{Hf}(\text{CO})_6]^{2-}$, $[\text{Ta}(\text{CO})_6]^-$, $\text{W}(\text{CO})_6$, $[\text{Re}(\text{CO})_6]^+$, $[\text{Os}(\text{CO})_6]^{2+}$, and $[\text{Ir}(\text{CO})_6]^{3+}$: A Theoretical Study. <i>Organometallics</i> , 1997, 16, 4807-4815. | 1.1 | 128 |
| 361 | Ab Initio Density Functional Calculations of Deuterium Kinetic Isotope Effects for Decomposition of Dimethylnitramine. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1370-1373. | 1.1 | 22 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 362 | Density Functional Study of ⁵⁹ Co Chemical Shielding Tensors Using Gauge-Including Atomic Orbitals. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3637-3640. | 1.1 | 21 |
| 363 | Theoretical Model for Insertion of the 16-Electron Species (Î-5-C5H5)M(L) into Saturated Hydrocarbons. A (Î-5-C5H5)M(CO) + CH4 (M = Ru-, Os-, Rh, Ir, Pd+, Pt+) Case Study. <i>Organometallics</i> , 1997, 16, 1621-1627. | 1.1 | 37 |
| 364 | Fluorescence Lifetime Measurements and Spectral Analysis of Adamantylidiazirine. <i>Journal of the American Chemical Society</i> , 1997, 119, 3580-3591. | 6.6 | 51 |
| 365 | Importance of Quantum Effects for C- ¹ H Bond Activation Reactions. <i>Journal of the American Chemical Society</i> , 1997, 119, 9891-9896. | 6.6 | 62 |
| 366 | Theoretical Characterization of an Intermediate for the [3 + 2] Cycloaddition Mechanism in the Bis(dihydroxy-quinidine)-3,6-Pyridazine- Λ -Osmium Tetroxide-Catalyzed Dihydroxylation of Styrene. <i>Journal of Organic Chemistry</i> , 1997, 62, 7892-7894. | 1.7 | 27 |
| 367 | Gas-Phase Reactions of Fe(CH2O)+ and Fe(CH2S)+ with Small Alkanes: An Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 1997, 119, 12879-12888. | 6.6 | 16 |
| 368 | Theoretical Study of M+ ⁺ CO ₂ and OM+CO Systems for First Transition Row Metal Atoms. <i>Journal of Physical Chemistry A</i> , 1997, 101, 7854-7859. | 1.1 | 112 |
| 369 | A DFT Study of the Simmons-Smith Cyclopropanation Reaction. <i>Journal of the American Chemical Society</i> , 1997, 119, 12300-12305. | 6.6 | 59 |
| 370 | Carbonyl Hypofluorite-A Density Functional Theoretical Study. <i>Journal of Physical Chemistry A</i> , 1997, 101, 9745-9748. | 1.1 | 4 |
| 371 | Pt+-Catalyzed Oxidation of Methane: Theory and Experiment. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1567-1579. | 1.1 | 156 |
| 372 | Synergy of Theory and Experiment in the Remote Functionalization of Aliphatic Nitriles by α -Bare-Fe(I) and Co(I) Cations in the Gas Phase. <i>Organometallics</i> , 1997, 16, 3135-3147. | 1.1 | 26 |
| 373 | Vibrational Transition Moments of Aminopurines: Stretched Film IR Linear Dichroism Measurements and DFT Calculations. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4361-4374. | 1.1 | 19 |
| 374 | Tautomeric Rearrangements in Mono- and Dichalcogenide Analogs of Formic Acid, HC(X)YH (X, Y = O, S). <i>Journal of Physical Chemistry A</i> , 1997, 101, 10000-10000. | 1.1 | 38 |
| 375 | Hartree-Fock and Density Functional Methods and IR and NMR Spectroscopies in the Examination of Tautomerism and Features of Neutral 9-Acridinamine in Gaseous and Condensed Media. <i>Journal of Physical Chemistry A</i> , 1997, 101, 283-292. | 1.1 | 39 |
| 376 | Static Dipole Polarizabilities through Density Functional Methods. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4231-4235. | 1.1 | 32 |
| 377 | Electronic Structure of the BF ₂ Radical Determined by ab Initio Calculations and Resonance-Enhanced Multiphoton Ionization Spectroscopy. <i>Journal of Physical Chemistry A</i> , 1997, 101, 2045-2049. | 1.1 | 11 |
| 378 | Binding energies of Ti+(H ₂) ₁₋₆ clusters: Theory and experiment. <i>Journal of Chemical Physics</i> , 1997, 106, 10153-10167. | 1.2 | 48 |
| 379 | A Computational Analysis of Substituent Effects on the O-H Bond Dissociation Energy in Phenols: Polar Versus Radical Effects. <i>Journal of the American Chemical Society</i> , 1997, 119, 4239-4244. | 6.6 | 170 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 380 | Mechanism of Acid-Catalyzed Epoxidation of Alkenes with Peroxy Acids. <i>Journal of Organic Chemistry</i> , 1997, 62, 5191-5197. | 1.7 | 79 |
| 381 | Ab Initio and Density Functional Study of 1,2-Sulfur Heterocycles. <i>Journal of Organic Chemistry</i> , 1997, 62, 1766-1774. | 1.7 | 30 |
| 382 | Density Functional Calculations of Structures, Vibrational Frequencies, and Normal Modes of trans- and cis-Azobenzene. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5555-5566. | 1.1 | 158 |
| 383 | An orbital-based density difference index for the comparison of electron density distributions. <i>Journal of Chemical Physics</i> , 1997, 107, 6693-6698. | 1.2 | 3 |
| 384 | Experimental and Theoretical Studies of SiFn(CO) ₂ + Cations with n = 2 and 3: A Search for Pentacoordinate Cationic Silicon. <i>Journal of Physical Chemistry A</i> , 1997, 101, 7258-7264. | 1.1 | 7 |
| 385 | Three-Electron SN ₂ Reactions of Arylcyclopropane Cation Radicals. 2. Steric and Electronic Effects of Substitution. <i>Journal of the American Chemical Society</i> , 1997, 119, 994-1004. | 6.6 | 72 |
| 386 | A Quantum Chemical Study of Hydrogen Abstraction from Manganese-Coordinated Water by a Tyrosyl Radical: A Model for Water Oxidation in Photosystem II. <i>Journal of the American Chemical Society</i> , 1997, 119, 8285-8292. | 6.6 | 124 |
| 387 | Density-Functional Studies on the Structure and Vibrational Spectra of Transient Intermediates of p-Benzoquinone. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4449-4459. | 1.1 | 72 |
| 388 | Structures and Vibrational Spectra of p-Benzoquinone in Different Oxidation and Protonation States: A Density Functional Study. <i>Journal of Physical Chemistry B</i> , 1997, 101, 1235-1246. | 1.2 | 44 |
| 389 | Ab Initio Calculations of the Ground Electronic States of Polyiodide Anions. <i>Journal of Physical Chemistry A</i> , 1997, 101, 2192-2197. | 1.1 | 72 |
| 390 | Understanding the activation energy trends for the C ₂ H ₄ +OH ⁺ →C ₂ H ₄ OH reaction by using canonical variational transition state theory. <i>Journal of Chemical Physics</i> , 1997, 107, 7266-7274. | 1.2 | 50 |
| 391 | Conformational Information from Vibrational Spectra of Styrene, trans-Stilbene, and cis-Stilbene. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3823-3831. | 1.1 | 291 |
| 392 | Rearrangements of C ₇ H ₆ Isomers: Computational Studies of the Interconversions of Bicyclo[3.2.0]hepta-1,3,6-triene, Bicyclo[3.2.0]hepta-3,6-diene-2-ylidene, Bicyclo[3.2.0]hepta-2,3,6-triene, and Cyclohepta-1,2,4,6-tetraene. <i>Journal of Organic Chemistry</i> , 1997, 62, 4398-4405. | 1.7 | 38 |
| 393 | Structures and Properties of Ubiquinone-1 and Its Radical Anion from Hybrid Hartree-Fock/Density Functional Studies. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5799-5804. | 1.1 | 36 |
| 394 | A new gradient-corrected exchange-correlation density functional. <i>Molecular Physics</i> , 1997, 91, 847-860. | 0.8 | 18 |
| 395 | Calculation of ionization energies, electron affinities, electronegativities, and hardnesses using density functional methods. <i>Journal of Chemical Physics</i> , 1997, 106, 3270-3279. | 1.2 | 142 |
| 396 | INFRARED AND RAMAN VIBRATIONAL OPTICAL ACTIVITY: Theoretical and Experimental Aspects. <i>Annual Review of Physical Chemistry</i> , 1997, 48, 357-386. | 4.8 | 298 |
| 397 | Organometallic Analogs of the Cyclobutadiene Dication: An Ab Initio MO and Density Functional Study of the Symmetrical Planar and Puckered [W _L 2(1/4-CR)] ₂ Complexes (L = H, Me, F, OH; R = H, F, Me). <i>Organometallics</i> , 1997, 16, 1425-1429. | 1.1 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 398 | Calculated One-Electron Reduction Potentials and Solvation Structures for Selected p-Benzoquinones in Water. <i>Journal of Physical Chemistry B</i> , 1997, 101, 623-631. | 1.2 | 65 |
| 399 | Theoretical investigation of the potential energy surface for the NH ₂ +NO reaction via density functional theory and ab initio molecular electronic structure theory. <i>Journal of Chemical Physics</i> , 1997, 106, 9236-9251. | 1.2 | 30 |
| 400 | Reactions of Laser-Ablated Scandium Atoms with Dioxygen. Infrared Spectra of ScO, OScO, (O ₂)ScO, (ScO) ₂ , and Sc(O ₂) ₂ in Solid Argon. <i>Journal of Physical Chemistry A</i> , 1997, 101, 9085-9091. | 1.1 | 69 |
| 401 | Reactions of Laser-Ablated Cobalt Atoms with O ₂ . Infrared Spectra of Cobalt Oxides in Solid Argon. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8793-8802. | 1.1 | 73 |
| 402 | Structures and potential energy surface of faujasitic zeolite/water. <i>Chemical Physics</i> , 1997, 215, 77-87. | 0.9 | 23 |
| 403 | Energetics, Kinetics, and Product Distributions of the Reactions of Ozone with Ethene and 2,3-Dimethyl-2-butene. <i>Journal of Physical Chemistry A</i> , 1997, 101, 9421-9429. | 1.1 | 202 |
| 404 | Single-Step and Multistep Mechanisms of Aromatic Nucleophilic Substitution of Halobenzenes and Halonitrobenzenes with Halide Anions: A Ab Initio Computational Study. <i>Journal of Organic Chemistry</i> , 1997, 62, 4036-4046. | 1.7 | 73 |
| 405 | Application of quantum-chemical methods including density functional theory for the interpretation of isotropic hyperfine data. The example of azulenebenzoquinone. <i>Applied Magnetic Resonance</i> , 1997, 13, 405-413. | 0.6 | 0 |
| 406 | Scaled quantum mechanical and experimental vibrational spectra of magnesium and zinc porphyrins. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1997, 53, 1195-1209. | 2.0 | 66 |
| 407 | The calculation of accurate harmonic frequencies of large molecules: the polycyclic aromatic hydrocarbons, a case study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1997, 53, 1225-1240. | 2.0 | 172 |
| 408 | Vibrational analysis of the spectra of furan and thiophene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1997, 53, 1365-1373. | 2.0 | 51 |
| 409 | On the cleavage of the peroxide O—O bond in methyl hydroperoxide and dimethyl peroxide upon protonation. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1997, 163, 101-119. | 1.9 | 20 |
| 410 | Theoretical and experimental investigations of the electronic circular dichroism and absorption spectra of bicyclic ketones. <i>Chemical Physics</i> , 1997, 224, 143-155. | 0.9 | 90 |
| 411 | Oxidative addition of mono and bis(carbene) complexes derived from imidazolyl and thiazolyl gold(I) compounds. <i>Journal of Organometallic Chemistry</i> , 1997, 544, 91-100. | 0.8 | 68 |
| 412 | To Couple or Not To Couple: The Dilemma of Acetylide Carbons in [(η^5 -C ₅ H ₅) ₂ M(η^4 -CCR) ₂ M(η^5 -C ₅ H ₅) ₂] Complexes (M = $\frac{3}{4}$ Ti, Zr) A Theoretical Study for R = $\frac{3}{4}$ H, F. <i>Angewandte Chemie International Edition in English</i> , 1997, 36, 606-608. | 4.4 | 40 |
| 413 | On the Mechanism of the McMurry Reaction. <i>Angewandte Chemie International Edition in English</i> , 1997, 36, 2234-2237. | 4.4 | 30 |
| 414 | Stabilization of Atomic Nitrogen Inside C ₆₀ . <i>Angewandte Chemie International Edition in English</i> , 1997, 36, 2835-2838. | 4.4 | 122 |
| 415 | Kuppeln, ja oder nein? â€” das Dilemma von Acetylidkohlenstoffzentren in [(η^5 -C ₅ H ₅) ₂ M(η^4 -CCR) ₂ M(η^5 -C ₅ H ₅) ₂] Complexes (M = Ti, Zr); eine theoretische Untersuchung fÃ¼r R = H, F. <i>Angewandte Chemie</i> , 1997, 109, 633-635. | 4.4 | 114 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 416 | Stabilisierung von atomarem Stickstoff im Innenraum von C ₆₀ . Angewandte Chemie, 1997, 109, 2858-2861. | 1.6 | 26 |
| 417 | A DFT Study on the Vinylcyclopropanecarbaldehyde-2,5-Dihydrooxepin Hetero-Cope Rearrangement and on Related Reactions. Liebigs Annalen, 1997, 1997, 2443-2449. | 0.8 | 26 |
| 418 | Comparison of different ab initio theoretical models for calculating isodesmic reaction energies for small ring and related compounds. Journal of Computational Chemistry, 1997, 18, 108-114. | 1.5 | 74 |
| 419 | Molecular energies and properties from density functional theory: Exploring basis set dependence of Kohn-Sham equation using several density functionals. Journal of Computational Chemistry, 1997, 18, 775-795. | 1.5 | 140 |
| 420 | High-level ab initio versus DFT calculations on (H ₂ O) ₂ and H ₂ O ₂ -H ₂ O complexes as prototypes of multiple hydrogen bond systems. , 1997, 18, 1124-1135. | | 127 |
| 421 | Ab initio study on the thermochemistry of diphosphine (P ₂ H ₄) and diphosphine radical cation (P ₂ H ₄ ⁺). Chemical Physics Letters, 1997, 265, 514-520. | 1.2 | 9 |
| 422 | Formic acid tetramers: structure isomers in the gas phase. Chemical Physics Letters, 1997, 267, 111-115. | 1.2 | 29 |
| 423 | On the parameterization of the local correlation functional. What is Becke-3-LYP?. Chemical Physics Letters, 1997, 268, 345-351. | 1.2 | 865 |
| 424 | A CCSD(T) and DFT investigation of m-benzyne and 4-hydroxy-m-benzyne. Chemical Physics Letters, 1997, 268, 313-320. | 1.2 | 70 |
| 425 | Methylene-iodonium ylide: an isomer of diiodomethane. Chemical Physics Letters, 1997, 269, 145-150. | 1.2 | 28 |
| 426 | Investigation of the use of B3LYP zero-point energies and geometries in the calculation of enthalpies of formation. Chemical Physics Letters, 1997, 270, 419-426. | 1.2 | 173 |
| 427 | The successive OH binding energies of Sc(OH) _n ⁺ for n = 1-3. Chemical Physics Letters, 1997, 272, 127-131. | 1.2 | 11 |
| 428 | Displacement energies for nanorods. Chemical Physics Letters, 1997, 273, 195-198. | 1.2 | 0 |
| 429 | Cost effective calculation of molecular charge distributions and gas phase deprotonation energies using density functional methods. Chemical Physics Letters, 1997, 274, 396-404. | 1.2 | 8 |
| 430 | Accurate theoretical structures of radical cations containing unusually long bonds: the structures of CH ₃ CH ₂ OH ⁺ , ÅH ₂ CH ₂ O+H ₂ . Chemical Physics Letters, 1997, 275, 28-34. | 1.2 | 28 |
| 431 | Trimesitylsilylium cation verification of a free silylium cation in solution by NMR chemical shift calculations. Chemical Physics Letters, 1997, 279, 9-16. | 1.2 | 16 |
| 432 | The calculation of frequency-dependent polarizabilities using current density functional theory. Chemical Physics Letters, 1997, 278, 278-284. | 1.2 | 50 |
| 433 | Time-dependent density functional theory applied to Raman scattering from methane. Chemical Physics Letters, 1997, 279, 17-21. | 1.2 | 13 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 434 | Computational study of the (CH ₃ Zn) ₂ B ₃ H ₇ and CH ₃ ZnBH ₄ dimers. Chemical Physics Letters, 1997, 280, 273-279. | 1.2 | 1 |
| 435 | Methylated NF ₃ . A G2MS theoretical study on the structure, stability, and interconversion of the CH ₃ â€“NF ₃ ⁺ and CH ₃ Fâ€“NF ₂ ⁺ isomers. Chemical Physics Letters, 1997, 281, 431-437. | 1.2 | 20 |
| 436 | The heats of formation of SiCln ⁺ , for n = 1â€“4. Chemical Physics Letters, 1997, 276, 47-54. | 1.2 | 3 |
| 437 | Water clusters studied by electrospray mass spectrometry. Journal of Chromatography A, 1997, 777, 155-165. | 1.8 | 41 |
| 438 | The Sc+â€“OH and Sc+â€“OCH ₃ bond energies in ScOH ⁺ , ScOCH ₃ ⁺ , Sc(OH) ₂ ⁺ , ScOHOCH ₃ ⁺ , and Sc(OCH ₃) ₂ ⁺ . Chemical Physics Letters, 1998, 284, 308-312. | 1.2 | 2 |
| 439 | The prediction of vibrational frequencies of inorganic molecules using density functional theory. Chemical Physics Letters, 1998, 282, 219-226. | 1.2 | 168 |
| 440 | Empirical density functionals. Chemical Physics Letters, 1998, 284, 6-11. | 1.2 | 95 |
| 441 | Density functional studies of the potential energy surface of the Ni+(CF ₃) complex. Chemical Physics Letters, 1998, 284, 339-343. | 1.2 | 8 |
| 442 | Accurate heats of formation for PHn, PHn ⁺ , and PHn ^{âˆš} . Chemical Physics Letters, 1998, 285, 455-458. | 1.2 | 13 |
| 443 | Ab initio study of ionic solutions by a polarizable continuum dielectric model. Chemical Physics Letters, 1998, 286, 253-260. | 1.2 | 1,493 |
| 444 | A density functional study of the internal rotation in the quadruply bonded Mo ₂ Cl ₄ (PH ₃) ₄ complex. Chemical Physics Letters, 1998, 287, 243-249. | 1.2 | 16 |
| 445 | Theoretical study of the radiationless decay channels of triplet state norbornene. Chemical Physics Letters, 1998, 287, 601-607. | 1.2 | 10 |
| 446 | Theoretical study of the structure and stability of Nb _x O _y and Nb _x O _y ⁺ (x=1â€“3; y=2â€“5,â€“7,â€“8) clusters. Chemical Physics Letters, 1998, 287, 620-626. | 1.2 | 36 |
| 447 | Calculation of adsorption energies of molecules in cages: a density functional approach. Chemical Physics Letters, 1998, 288, 628-634. | 1.2 | 11 |
| 448 | A combined experimental far-infrared and computational density functional approach applied to aluminum-alkyl cocatalysts. Chemical Physics Letters, 1998, 290, 99-104. | 1.2 | 10 |
| 449 | Static and dynamic polarisabilities, Cauchy coefficients and their anisotropies: a comparison of standard methods. Chemical Physics Letters, 1998, 291, 71-77. | 1.2 | 45 |
| 450 | Towards linear scaling in continuum solvent models.. Chemical Physics Letters, 1998, 293, 221-229. | 1.2 | 34 |
| 451 | A CASSCF/ACPF study of spectroscopic properties of FeS and FeS ^{âˆš} and the photoelectron spectrum of FeS ^{âˆš} . Chemical Physics Letters, 1998, 294, 37-44. | 1.2 | 37 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 452 | Heats of formation for NFn ($n=1-3$) and NFn^+ ($n=1-3$). <i>Chemical Physics Letters</i> , 1998, 294, 454-458. | 1.2 | 17 |
| 453 | Tests of a density functional with Laplacian terms: activation barriers and bond-stretching energies. <i>Chemical Physics Letters</i> , 1998, 295, 467-474. | 1.2 | 15 |
| 454 | Intermolecular ReH_5 , H_2 , H_2 , X hydrogen bonding ($X = N, C$) involving $ReH_5(PPh_3)_3$. <i>Inorganica Chimica Acta</i> , 1998, 280, 26-29. | 1.2 | 15 |
| 455 | Hybrid methods: Combining density functional and wavefunction theory. , 1998, , 60-90. | | 5 |
| 456 | New Class IV Charge Model for Extracting Accurate Partial Charges from Wave Functions. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1820-1831. | 1.1 | 259 |
| 457 | Assessment of Gaussian-2 and density functional theories for the computation of ionization potentials and electron affinities. <i>Journal of Chemical Physics</i> , 1998, 109, 42-55. | 1.2 | 536 |
| 458 | Proton transfer between carbon acids and methoxide: Studies in methanol, the gas phase and by ab initio MO calculations. <i>Zeitschrift Fur Elektrotechnik Und Elektrochemie</i> , 1998, 102, 567-572. | 0.9 | 5 |
| 459 | Cis,trans,cis or All-cis Geometry in d ⁰ Octahedral Dioxo Complexes. An IMOMM Study of the Role of Steric Effects. <i>Inorganic Chemistry</i> , 1998, 37, 3321-3325. | 1.9 | 28 |
| 460 | A comparison of electron transfer in ribonucleotide reductase and the bacterial photosynthetic reaction center. <i>Chemical Physics Letters</i> , 1998, 292, 421-430. | 1.2 | 30 |
| 461 | The use of density functional theory-based reactivity descriptors in molecular similarity calculations. <i>Chemical Physics Letters</i> , 1998, 295, 122-128. | 1.2 | 37 |
| 462 | Organometallic clusters: What is an appropriate DFT treatment?. <i>Journal of Organometallic Chemistry</i> , 1998, 565, 271-277. | 0.8 | 14 |
| 463 | Infrared spectra of polycyclic aromatic hydrocarbons: methyl substitution and loss of H. <i>Chemical Physics</i> , 1998, 234, 79-86. | 0.9 | 18 |
| 464 | Deuterium depth profiling in polymers using heavy ion elastic recoil detection. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1998, 134, 237-248. | 0.6 | 10 |
| 465 | Comparison of density functional and MP2 geometry optimizations of $Na(H_2O)_n$ ($n = 1-3$) clusters. <i>Computational and Theoretical Chemistry</i> , 1998, 425, 87-94. | 1.5 | 6 |
| 466 | Hybrid Hartree-Fock/density functional (HF/DF) calculations of adiabatic electron affinities (EA _{ad} 's) of neutral hydroquinone radicals of 1,4-benzoquinone (1) and 1,4-benzoquinone imine (2). <i>Computational and Theoretical Chemistry</i> , 1998, 454, 237-258. | 1.5 | 10 |
| 467 | An electronic structure investigation of the BNO-BON-NBO system. <i>Computational and Theoretical Chemistry</i> , 1998, 430, 137-148. | 1.5 | 12 |
| 468 | Novel Nine-Membered Titanaheterocycles – Structure, ab initio Calculations, and Preparative Use towards the Selective Synthesis of Substituted Cyclopentanols. <i>European Journal of Inorganic Chemistry</i> , 1998, 1998, 1253-1262. | 1.0 | 6 |
| 469 | Theoretical Comparison of the Electronic Structures of $[PhN_2]^+$ and $[PhP_2]^+$ – Can the Benzenediphosphonium Cation Exist in the Gas Phase?. <i>European Journal of Inorganic Chemistry</i> , 1998, 1998, 1821-1825. | 1.0 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 470 | A Combined Neutralization-Reionization Mass Spectrometric and Theoretical Study of Oxyallyl and Other Elusive [C3, H4, O] Neutrals. <i>European Journal of Organic Chemistry</i> , 1998, 1998, 987-1009. | 1.2 | 34 |
| 471 | Structure/Chiroptics Relationships of Planar Chiral and Helical Molecules. <i>European Journal of Organic Chemistry</i> , 1998, 1998, 1491-1509. | 1.2 | 208 |
| 472 | Multichromophoric Systems by Diels-Alder Reaction of Barrelene witho-Benzoquinones: Tetracyclo[6.2.2.2.3,6.02,7]tetradeca-9,11,13-triene-4,5-diones. <i>European Journal of Organic Chemistry</i> , 1998, 1998, 2339-2348. | 1.2 | 5 |
| 473 | On the use of ultraviolet resonance Raman intensities to elaborate molecular force fields: Application to nucleic acid bases and aromatic amino acid residues models. , 1998, 4, 379-393. | | 6 |
| 476 | Protonation enthalpies in fluorosulfonic acid using ab initio self-consistent reaction field theory. <i>Journal of Computational Chemistry</i> , 1998, 19, 250-257. | 1.5 | 11 |
| 477 | Geometry optimization of molecular structures in solution by the polarizable continuum model. <i>Journal of Computational Chemistry</i> , 1998, 19, 404-417. | 1.5 | 1,602 |
| 478 | Inexpensive vibrational anharmonicities from estimated derivatives: Diatomic molecules. <i>Journal of Computational Chemistry</i> , 1998, 19, 1315-1324. | 1.5 | 7 |
| 479 | Theoretical study of structure of alkali metal cyanates and isocyanates and their related ion pair SN2 reactions. <i>Journal of Computational Chemistry</i> , 1998, 19, 1325-1336. | 1.5 | 21 |
| 480 | QCISD(T) and B3LYP can correctly describe the EA of B, Al, and Ga. <i>International Journal of Quantum Chemistry</i> , 1998, 66, 285-286. | 1.0 | 3 |
| 481 | Difficulties of density functional theory in predicting the torsional potential of 2,2'-bithiophene. , 1998, 70, 303-312. | | 34 |
| 482 | Singlet-triplet splitting and the activation of C-H bond for (5-C5H5)M(CO) isoelectronic fragments: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 1998, 70, 961-971. | 1.0 | 8 |
| 483 | Mechanism of methane monooxygenase - a structural and quantum chemical perspective. <i>Journal of Biological Inorganic Chemistry</i> , 1998, 3, 314-317. | 1.1 | 61 |
| 484 | IR spectrum and normal mode analysis of the anti-Alzheimer's disease natural product Huperzine A: A quantum chemistry density-functional theory (DFT) investigation. <i>Science in China Series B: Chemistry</i> , 1998, 41, 616-622. | 0.8 | 4 |
| 485 | Analysis of the polarized Raman spectra of 9-methylfluoren-9-ol crystal: vibrational assignments. <i>Journal of Molecular Structure</i> , 1998, 441, 27-38. | 1.8 | 0 |
| 486 | Methylzinc tetrahydroborate: investigation of the vapour phase by spectroscopic and quantum chemical techniques. <i>Journal of Molecular Structure</i> , 1998, 444, 29-46. | 1.8 | 5 |
| 487 | Vibrational spectra and conformations of 1,4-cyclohexadiene and its oxygen analogues: ab initio and density functional calculations. <i>Journal of Molecular Structure</i> , 1998, 470, 265-275. | 1.8 | 8 |
| 488 | Generation of neutral and cationic hydrogen shift isomers of pyridine: a combined experimental and computational investigation. <i>International Journal of Mass Spectrometry</i> , 1998, 179-180, 7-14. | 0.7 | 54 |
| 489 | Post-Hartree-Fock MP2 and density functional theory derived structure and vibrations of 1,2-dithiole-2-thione and 1,2-dithiole-3-one. <i>Vibrational Spectroscopy</i> , 1998, 16, 77-83. | 1.2 | 11 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 490 | Vibrational circular dichroism spectroscopy of chiral pheromones: frontalin (1,5-dimethyl-6,8-dioxabicyclo[3.2.1]octane). <i>Tetrahedron: Asymmetry</i> , 1998, 9, 1107-1110. | 1.8 | 45 |
| 491 | Theoretical study of structures, energetics and vibrational properties of BC ₂ H ₃ species. <i>Chemical Physics</i> , 1998, 230, 143-151. | 0.9 | 13 |
| 492 | Infrared spectra of polycyclic aromatic hydrocarbons: nitrogen substitution. <i>Chemical Physics</i> , 1998, 234, 87-94. | 0.9 | 29 |
| 493 | Infrared spectra of polycyclic aromatic hydrocarbons: oxygen substitution. <i>Chemical Physics</i> , 1998, 233, 29-34. | 0.9 | 14 |
| 494 | Matrix photochemistry of nitrosyl chloride.. <i>Chemical Physics</i> , 1998, 237, 251-264. | 0.9 | 26 |
| 495 | Protonated NF ₃ O. A G ₂ MS theoretical study on the structure, stability, and interconversion of the (NF ₃ O)H ⁺ isomers. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1998, 175, 317-324. | 1.9 | 4 |
| 496 | On the helical conformation of un-ionized poly(¹³ -d-glutamic acid). <i>International Journal of Biological Macromolecules</i> , 1998, 23, 175-184. | 3.6 | 55 |
| 497 | Accurate Heats of Formation for SF _n , SF _n ⁺ , and SF _n -form= 1 [~] 6. <i>Journal of Physical Chemistry A</i> , 1998, 102, 4722-4727. | 1.1 | 66 |
| 498 | Molecular and Electronic Structures of Heteroaromatic Oligomers: A Model Compounds of Polymers with Quantum-Well Structures. <i>Journal of Organic Chemistry</i> , 1998, 63, 1041-1048. | 1.7 | 57 |
| 499 | Reactivity of diatomic molecules on Cu(100). <i>Surface Science</i> , 1998, 417, 247-260. | 0.8 | 28 |
| 500 | Femtosecond Activation of Reactions and the Concept of Nonergodic Molecules. <i>Science</i> , 1998, 279, 847-851. | 6.0 | 153 |
| 501 | Theoretical Investigation of Two-State-Reactivity Pathways of H ⁺ Activation by FeO ⁺ : A Addition~Elimination, a~Rebound~, and Oxene-Insertion Mechanisms. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3835-3846. | 1.1 | 145 |
| 502 | Do bond functions help for the calculation of accurate bond energies?. <i>Journal of Chemical Physics</i> , 1998, 109, 4707-4712. | 1.2 | 15 |
| 503 | Binding of dioxygen in a picket-fence porphyrin complex of iron. A theoretical QM/MM study. <i>New Journal of Chemistry</i> , 1998, 22, 327-322. | 1.4 | 22 |
| 504 | A High-Level Computational Study on the Thermochemistry and Thermal Decomposition of Sulfur Mustard (2,2~Dichloroethyl Sulfide): a~ A Chemical Warfare Agent. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3438-3446. | 1.1 | 14 |
| 505 | Accurate Heats of Formation for SiF _n and SiF _n ⁺ , for n = 1 [~] 4. <i>Journal of Physical Chemistry A</i> , 1998, 102, 876-880. | 1.1 | 37 |
| 506 | Infrared and Raman Spectroscopy of Bis(4,4-dimethyl-2,5-cyclohexadien-1-ylidene). Vibrational Assignment by Hartree~Fock and Density Functional Theory Calculations and Depolarization Method. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2679-2684. | 1.1 | 2 |
| 507 | Heats of Formation of GaCl ₃ and Its Fragments. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10424-10429. | 1.1 | 16 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 508 | Hydration of Beryllium, Magnesium, Calcium, and Zinc Ions Using Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 1998, 102, 219-228. | 1.1 | 487 |
| 509 | A conformational study of (1S, 2R, 5S)-(+)-menthol using vibrational circular dichroism spectroscopy. <i>Canadian Journal of Chemistry</i> , 1998, 76, 274-283. | 0.6 | 23 |
| 510 | Breaking an electronically preferred symmetry by steric effects in a series of [Ir(biph)X(QR3)2] compounds (X=Cl or I, Q=P or As). <i>New Journal of Chemistry</i> , 1998, 22, 1493-1498. | 1.4 | 22 |
| 511 | Phosphines exchange in quadruply bonded metal dimers: theoretical proposal for an alternative to the internal flip mechanism. <i>Chemical Communications</i> , 1998, , 1443-1444. | 2.2 | 8 |
| 512 | Opposing steric and electronic contributions in OsCl2H2(PPr3i)2. A theoretical study of an unusual structure. <i>New Journal of Chemistry</i> , 1998, 22, 5-9. | 1.4 | 34 |
| 513 | Potential energy function and vibrational states of HN3 and DN3. <i>Molecular Physics</i> , 1998, 93, 853-865. | 0.8 | 2 |
| 514 | Electronic Spectra of Phenylcyclopropane and Cumene Cation Radicals: An Interplay of Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 1998, 102, 8979-8987. | 1.1 | 11 |
| 515 | Nitrogen Fixation by Nitrogenases: A Quantum Chemical Study. <i>Journal of Physical Chemistry B</i> , 1998, 102, 1615-1623. | 1.2 | 97 |
| 516 | Computational Study on the Thermochemistry of Cyclopentadiene Derivatives and Kinetics of Cyclopentadienone Thermal Decomposition. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1530-1541. | 1.1 | 71 |
| 517 | Ring Opening of the Cyclopropylcarbinyl Radical and Its N- and O-Substituted Analogues: A Theoretical Examination of Very Fast Unimolecular Reactions. <i>Journal of the American Chemical Society</i> , 1998, 120, 10223-10233. | 6.6 | 96 |
| 518 | Theoretical Study on X-H, -O, -OH, -NO, -ONO, and -NO2 (X = CH3, t-C4H9, C13H21). <i>Journal of Physical Chemistry A</i> , 1998, 102, 2002-2008. | 1.1 | 10 |
| 519 | Atomization Energies of SO and SO2: Basis Set Extrapolation Revisited. <i>Journal of Physical Chemistry A</i> , 1998, 102, 8044-8050. | 1.1 | 58 |
| 520 | Comparative ab Initio Study of Molecular Structures and Relative Stabilities of Germanone, Germathione, Germaselenone, and Their Structural Isomers. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2189-2193. | 1.1 | 18 |
| 521 | Gas-Phase Chemistry of NHxCl _y ⁺ . 1. Structure, Stability, and Reactivity of Protonated Monochloramine. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10189-10194. | 1.1 | 16 |
| 522 | Elemental Chlorine and Chlorine Fluoride: Theoretical and Experimental Proton Affinity and the Gas Phase Chemistry of Cl2H ⁺ and FClH ⁺ Ions. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10560-10567. | 1.1 | 11 |
| 523 | Theoretical Study of the Substrate Mechanism of Ribonucleotide Reductase. <i>Journal of the American Chemical Society</i> , 1998, 120, 8417-8429. | 6.6 | 110 |
| 524 | Single versus Double Proton-Transfer Reactions in Watson-Crick Base Pair Radical Cations. A Theoretical Study. <i>Journal of the American Chemical Society</i> , 1998, 120, 8159-8167. | 6.6 | 203 |
| 525 | Synthesis and Characterization of OsX{NHC(Ph)C6H4}H2(PiPr3)2 (X = H, Cl, Br, I): Nature of the H2 Unit and Its Behavior in Solution. <i>Organometallics</i> , 1998, 17, 4065-4076. | 1.1 | 81 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 526 | Vibrational Absorption and Circular Dichroism of Mono- and Dimethyl Derivatives of 6,8-Dioxabicyclo[3.2.1]octane. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6842-6857. | 1.1 | 30 |
| 527 | Experimental and Theoretical Studies of MCF ₃ ⁺ (M = Fe and Co): Reactivities, Structures, and Potential Energy Surface for C-H Activation. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3343-3351. | 1.1 | 28 |
| 528 | Sequential Ligation of Mg ⁺ , Fe ⁺ , (c-C ₅ H ₅)Mg ⁺ , and (c-C ₅ H ₅)Fe ⁺ with Ammonia in the Gas Phase: Transition from Coordination to Solvation in the Sequential Ligation of Mg ⁺ . <i>Journal of Physical Chemistry A</i> , 1998, 102, 9803-9810. | 1.1 | 48 |
| 529 | Density Functional Theory Calculations on 19-Electron Organometallic Complexes: The Mn(CO) ₅ Cl ⁻ Anion. The Difference between Unpaired Electron Density and Spin Density Due to Spin Polarization. <i>Organometallics</i> , 1998, 17, 4060-4064. | 1.1 | 18 |
| 530 | Modeling Electron Transfer in Biochemistry: A Quantum Chemical Study of Charge Separation in Rhodospira rubra and Photosystem II. <i>Journal of the American Chemical Society</i> , 1998, 120, 8812-8824. | 6.6 | 207 |
| 531 | Gas Phase Reaction of Neutral Carbon Disulfide with Its Hydride Adduct Anions: Tandem Mass Spectrometry and Theoretical Studies. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3732-3737. | 1.1 | 9 |
| 532 | Effect of the Spinning Motion of the Dihydrogen Ligand on the Properties of an Elongated Dihydrogen Complex. A Theoretical Study of the trans-[Os(H ₂)(H)Cl(H ₂ PCH ₂ CH ₂ PH ₂) ₂] ⁺ Complex. <i>Journal of the American Chemical Society</i> , 1998, 120, 8168-8176. | 6.6 | 45 |
| 533 | Development of New Exchange-Correlation Functionals. 2. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3162-3168. | 1.1 | 43 |
| 534 | Inadequacies of the Point-Dipole Approximation for Describing Electron-Nuclear Interactions in Paramagnetic Proteins: Hybrid Density Functional Calculations and the Analysis of NMR Relaxation of High-Spin Iron(III) Rubredoxin. <i>Journal of Physical Chemistry B</i> , 1998, 102, 8300-8305. | 1.2 | 30 |
| 535 | A Crystallographic and Computational Study of a Diethyl Ether Complex of Fluorenyllithium. <i>Organometallics</i> , 1998, 17, 1208-1214. | 1.1 | 30 |
| 536 | 3,3-Didehydro-5-methyl-6-hydroxytoluene: Matrix Isolation of a Diradical Related to the Neocarzinostatin Chromophore. <i>Journal of the American Chemical Society</i> , 1998, 120, 8480-8485. | 6.6 | 33 |
| 537 | Isotope Exchange in Ionized O ₃ /O ₂ Mixtures: The Role of O ₅ ⁺ , a Unique O ₃ Complex. <i>Inorganic Chemistry</i> , 1998, 37, 1398-1400. | 1.9 | 11 |
| 538 | Infrared and Raman Spectroscopy of 9,9-Spirobifluorene, Bis(2,2'-biphenylene)silane, and Bis(2,2'-biphenylene)germane. Vibrational Assignment by Depolarization Measurement and HF and Density Functional Theory Studies. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1139-1145. | 1.1 | 13 |
| 539 | Hydrogen Atom Transfer in Ribonucleotide Reductase (RNR). <i>Journal of Physical Chemistry B</i> , 1998, 102, 10622-10629. | 1.2 | 138 |
| 540 | Mechanism of Anionic [3 + 2] Cycloadditions. An ab Initio Computational Study on the Cycloaddition of Allyl-, 2-Borylallyl-, and 2-Azaallyllithium to Ethylene. <i>Journal of the American Chemical Society</i> , 1998, 120, 3357-3370. | 6.6 | 34 |
| 541 | Four-Electron Reduction of Diazo Compounds at a Single Tungsten Metal Center: A Theoretical Study of the Mechanism. <i>Journal of the American Chemical Society</i> , 1998, 120, 6598-6602. | 6.6 | 21 |
| 542 | Infrared Spectra of Substituted Polycyclic Aromatic Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1632-1646. | 1.1 | 68 |
| 543 | A CCSD(T) Study of the Relative Stabilities of Cytosine Tautomers. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10813-10817. | 1.1 | 130 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 544 | A Quantum Chemical View on the Mechanism of the Ta ⁺ -Mediated Coupling of Carbon Dioxide with Methane. <i>Organometallics</i> , 1998, 17, 2344-2351. | 1.1 | 35 |
| 545 | Differentiating between H and F or H and CN on C(111) or Si(111) Surfaces. <i>Journal of Physical Chemistry B</i> , 1998, 102, 2403-2405. | 1.2 | 8 |
| 546 | Analysis of Permanent Electric Dipole Moments of Aliphatic Hydrocarbon Molecules. 2. DFT Results. <i>Journal of Chemical Information and Computer Sciences</i> , 1998, 38, 313-316. | 2.8 | 6 |
| 547 | Proton Affinity of Dimethyl Sulfoxide and Relative Stabilities of C ₂ H ₆ OS Molecules and C ₂ H ₇ OS ⁺ Ions. A Comparative G ₂ (MP2) <i>ab Initio</i> and Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 1998, 102, 4703-4713. | 1.1 | 131 |
| 548 | On the Origin of Substrate Directing Effects in the Epoxidation of Allyl Alcohols with Peroxyformic Acid. <i>Journal of the American Chemical Society</i> , 1998, 120, 680-685. | 6.6 | 50 |
| 549 | Synthesis and Spectroscopic and Theoretical Characterization of the Elongated Dihydrogen Complex OsCl ₂ (<i>η</i> -2-H ₂)(NHCPPh ₂)(P <i>i</i> Pr ₃) ₂ . <i>Inorganic Chemistry</i> , 1998, 37, 5033-5035. | 1.9 | 43 |
| 550 | Gas-Phase Syntheses of Three Isomeric C ₅ H ₂ Radical Anions and Their Elusive Neutrals. A Joint Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 1998, 102, 9949-9956. | 1.1 | 44 |
| 551 | Density Functional Calculations of 19-Electron Organometallic Molecules. A Comparison of Calculated and Observed Anisotropic Hyperfine Coupling Constants for the CpCo(CO) ₂ -Anion. Implications for Determining Orbital Spin Populations from EPR Data. <i>Journal of the American Chemical Society</i> , 1998, 120, 942-947. | 6.6 | 28 |
| 552 | A Quantum Chemical Investigation of the C ⁺ -O Bond Length and Stretching Mode of the Phenolate Anion. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10128-10133. | 1.1 | 24 |
| 553 | Density Functional Study of Excited Charge Transfer State Formation in 4-(N,N-Dimethylamino)benzonitrile. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6297-6306. | 1.1 | 98 |
| 554 | Matrix Infrared Study of O-Initiated Atomic Oxidation of CH ₃ Cl: Identification of the Triplet CH ₃ Cl ⁺ ·O Complex. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10221-10229. | 1.1 | 9 |
| 555 | Systematic Errors in <i>ab Initio</i> Bond Dissociation Energies. <i>Journal of Physical Chemistry A</i> , 1998, 102, 9031-9039. | 1.1 | 13 |
| 556 | Electrophilic and Oxidative Activation of the Central C ⁺ Bond in [3.3.n]Propellanes: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 1998, 63, 6494-6502. | 1.7 | 29 |
| 557 | Bonding and Geometry of OCF ₃ ⁻ , ONF ₃ , and Related Molecules in Terms of the Ligand Close Packing Model. <i>Inorganic Chemistry</i> , 1998, 37, 6884-6889. | 1.9 | 21 |
| 558 | On Pure Axial Monosubstituted Cyclohexanes. <i>Journal of the American Chemical Society</i> , 1998, 120, 12145-12146. | 6.6 | 7 |
| 559 | Theoretical Study of Stable Trans and Cis Isomers in [UO ₂ (OH) ₄] ₂ -Using Relativistic Density Functional Theory. <i>Inorganic Chemistry</i> , 1998, 37, 4442-4451. | 1.9 | 137 |
| 560 | Methane Activation by Naked Rh ⁺ Atoms. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 1998, 102, 7303-7307. | 1.1 | 37 |
| 561 | The Mechanism of the Gas-Phase Ion ⁺ Molecule Reaction between Al ⁺ and Ethanol. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10493-10500. | 1.1 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 562 | High-Level Computational Study of the Stereoelectronic Effects of Substituents on Alkene Epoxidations with Peroxyformic Acid. <i>Journal of the American Chemical Society</i> , 1998, 120, 9902-9910. | 6.6 | 65 |
| 563 | Energetics of Cation Radical Formation at the Proximal Active Site Tryptophan of Cytochrome c Peroxidase and Ascorbate Peroxidase. <i>Journal of Physical Chemistry B</i> , 1998, 102, 8221-8228. | 1.2 | 58 |
| 564 | Electron Energy Loss and DFT/SCI Study of the Singlet and Triplet Excited States and Electron Attachment Energies of Tetramethylsilane, Hexamethyldisilane, Tris(trimethylsilyl)silane, and Tetramethoxysilane. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3524-3531. | 1.1 | 15 |
| 565 | Dimerization of Carboxylic Acids: Reliability of Theoretical Calculations and the Effect of Solvent. <i>Journal of Physical Chemistry B</i> , 1998, 102, 2269-2276. | 1.2 | 80 |
| 566 | The Nature of the Transition Structure for the Oxidation of Alkanes with Dioxiranes. <i>Journal of the American Chemical Society</i> , 1998, 120, 10528-10533. | 6.6 | 60 |
| 567 | Cationic Gold(I) Complexes of Xenon and of Ligands Containing the Donor Atoms Oxygen, Nitrogen, Phosphorus, and Sulfur. <i>Inorganic Chemistry</i> , 1998, 37, 624-632. | 1.9 | 255 |
| 568 | Ab Initio Study of Hydrogen-Bonded Complexes of Small Organic Molecules with Water. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3782-3797. | 1.1 | 396 |
| 569 | Comparative ab Initio Treatment (Hartree-Fock, Density Functional Theory, MP2, and Quadratic Configuration Interaction) of the Ground State of the Hydrogen Molecule. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6993-7000. | 1.1 | 20 |
| 570 | Experimental and Theoretical Investigation of the Geometry and Vibrational Frequencies of 1,2,3-Triazole, 1,2,4-Triazole, and Tetrazole Anions. <i>Journal of Physical Chemistry A</i> , 1998, 102, 620-629. | 1.1 | 45 |
| 571 | Structure and Vibrational Spectra of the Zwitterion L-Alanine in the Presence of Explicit Water Molecules: A Density Functional Analysis. <i>Journal of Physical Chemistry B</i> , 1998, 102, 5899-5913. | 1.2 | 179 |
| 572 | Radical Addition to Alkenes: A Further Assessment of Theoretical Procedures. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2237-2245. | 1.1 | 147 |
| 573 | A DFT Investigation of Ethylene Dimerization Catalyzed by Ni(0) Complexes. <i>Journal of the American Chemical Society</i> , 1998, 120, 7770-7775. | 6.6 | 40 |
| 574 | Site of Protonation in Aniline and Substituted Anilines in the Gas Phase: A Study via the Local Hard and Soft Acids and Bases Concept. <i>Journal of Physical Chemistry A</i> , 1998, 102, 7035-7040. | 1.1 | 135 |
| 575 | Density Functional Theory: A Source of Chemical Concepts and a Cost-Effective Methodology for Their Calculation. <i>Advances in Quantum Chemistry</i> , 1998, 33, 303-328. | 0.4 | 118 |
| 576 | Ordered Structures in Polycarbonate Studied by Infrared and Raman Spectroscopy, Wide-Angle X-ray Scattering, and Differential Scanning Calorimetry. <i>Macromolecules</i> , 1998, 31, 6611-6619. | 2.2 | 68 |
| 577 | Computational Thermochemistry. <i>ACS Symposium Series</i> , 1998, , 2-18. | 0.5 | 21 |
| 578 | A comparison of ZnO and ZnO ⁺ . <i>Journal of Chemical Physics</i> , 1998, 109, 8430-8434. | 1.2 | 38 |
| 579 | Improving virtual Kohn-Sham orbitals and eigenvalues: Application to excitation energies and static polarizabilities. <i>Journal of Chemical Physics</i> , 1998, 109, 10180-10189. | 1.2 | 886 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 580 | Superacid-Catalyzed Electrocyclization of Diphenylmethyl Cations to Fluorenes. Kinetic and Theoretical Revisit Supporting the Involvement of Ethylene Dications. <i>Journal of the American Chemical Society</i> , 1998, 120, 4629-4637. | 6.6 | 27 |
| 581 | Ab Initio Study of the Solvent Effects on the Singlet-Triplet Gap of Nitrenium Ions and Carbenes. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2732-2738. | 1.1 | 46 |
| 582 | Oxidation of Alkenes, Sulfides, Amines, and Phosphines with Peroxynitrous Acid: A Comparison with Other Oxidants Such as Peroxyformic Acid and Dimethyldioxirane. <i>Journal of the American Chemical Society</i> , 1998, 120, 775-783. | 6.6 | 57 |
| 583 | Diminishing π -Stabilization of an Unsaturated Metal Center: Hydrogen Bonding to $\text{OsHCl}(\text{CO})(\text{PtBu}_2\text{Me})_2$. <i>Journal of the American Chemical Society</i> , 1998, 120, 12553-12563. | 6.6 | 36 |
| 584 | Mechanism of H^+ Activation by Nickel-Iron Hydrogenase. <i>Journal of the American Chemical Society</i> , 1998, 120, 548-555. | 6.6 | 173 |
| 585 | Theoretical Study of Aqueous N-Acetyl-L-alanine N-Methylamide: Structures and Raman, VCD, and ROA Spectra. <i>Journal of Physical Chemistry B</i> , 1998, 102, 2587-2602. | 1.2 | 261 |
| 586 | Origin of Bonding Interactions in $\text{Cu}^+(\text{H}_2)_n$ Clusters: An Experimental and Theoretical Investigation. <i>Journal of the American Chemical Society</i> , 1998, 120, 13494-13502. | 6.6 | 81 |
| 587 | Bond Lengths and Bond Angles in Oxo, Hydroxo, and Alkoxo Molecules of Be, B, and C: A Close-Packed Nearly Ionic Model. <i>Inorganic Chemistry</i> , 1998, 37, 2811-2825. | 1.9 | 43 |
| 588 | Size-consistent wave functions for nondynamical correlation energy: The valence active space optimized orbital coupled-cluster doubles model. <i>Journal of Chemical Physics</i> , 1998, 109, 10669-10678. | 1.2 | 222 |
| 589 | The Reaction of Polycyclic Aromatic Hydrocarbon Cations with Hydrogen Atoms: The Astrophysical Implications. <i>Astrophysical Journal</i> , 1998, 509, L125-L127. | 1.6 | 97 |
| 591 | Vibrational spectra of charged defects in a series of I^{\pm}_2 -dimethyl end-capped oligothiophenes induced by chemical doping with iodine. <i>Journal of Chemical Physics</i> , 1998, 109, 10419-10429. | 1.2 | 107 |
| 592 | Analytical second derivatives of the free energy in solution by polarizable continuum models. <i>Journal of Chemical Physics</i> , 1998, 109, 6246-6254. | 1.2 | 220 |
| 593 | Why semilocal functionals work: Accuracy of the on-top pair density and importance of system averaging. <i>Journal of Chemical Physics</i> , 1998, 109, 3760-3771. | 1.2 | 167 |
| 594 | The Thiosulfine-Dithiirane-Dithioester Manifold $R^{>1}</sup>R^{>2}</sup>(CS^{>2}</sub>). Sulfur Reports, 1998, 21, 1-42.$ | 0.7 | 31 |
| 595 | Theoretical Study of the Effect of a Lewis Acid on Hydrogen Exchange Coupling in a Trihydride Metallocene: The $\text{Cp}_2\text{NbH}_3\text{-AlH}_3$ System. <i>Inorganic Chemistry</i> , 1998, 37, 2334-2339. | 1.9 | 12 |
| 596 | Theoretical studies of the structures and vibrational frequencies of actinide compounds using relativistic effective core potentials with Hartree-Fock and density functional methods: UF_6 , NpF_6 , and PuF_6 . <i>Journal of Chemical Physics</i> , 1998, 109, 3875-3881. | 1.2 | 163 |
| 597 | Heats of Formation for GeH_n ($n=1-4$) and Ge_2H_n ($n=1-6$). <i>Journal of Physical Chemistry A</i> , 1999, 103, 11121-11125. | 1.1 | 41 |
| 598 | Can C-C Hoogsteen-wobble pairs contribute to the stability of $d(\text{G}\cdot\text{C-C})$ triplexes?. <i>Nucleic Acids Research</i> , 1999, 27, 2248-2255. | 6.5 | 17 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 599 | Crossed beams reaction of atomic carbon, C(3Pj), with d6-benzene, C6D6(XAŠ1A1g): Observation of the per-deutero-1,2-didehydro- cycloheptatrienyl radical, C7D5(XAŠ2B2). Journal of Chemical Physics, 1999, 110, 6091-6094. | 1.2 | 64 |
| 600 | Electron affinities of the first- and second-row atoms: Benchmarkab initioand density-functional calculations. Physical Review A, 1999, 60, 1034-1045. | 1.0 | 95 |
| 601 | Thermodynamical stability of CH3ONO and CH3ONO ^ˆ : A coupled-cluster and Hartree ^ˆ Fock-density-functional-theory study. Journal of Chemical Physics, 1999, 110, 403-411. | 1.2 | 31 |
| 602 | Vibrational study of a well ^ˆ barrier ^ˆ well thiophene ^ˆ based oligomer in relation to the effective I ^ˆ conjugation length. Journal of Chemical Physics, 1999, 110, 6907-6915. | 1.2 | 26 |
| 603 | Ligands with radical character for high oxidation states in manganese and iron complexes. Molecular Physics, 1999, 96, 571-581. | 0.8 | 10 |
| 604 | A class IV charge model for molecular excited states. Journal of Chemical Physics, 1999, 110, 724-733. | 1.2 | 50 |
| 605 | Gallium compounds, a possible problem for the G2 approaches. Journal of Chemical Physics, 1999, 110, 1879-1881. | 1.2 | 28 |
| 606 | Accurate dipole moments from Hartree ^ˆ Fock calculations by means of class IV charges. Journal of Chemical Physics, 1999, 111, 885-892. | 1.2 | 23 |
| 607 | Analytical free energy second derivatives with respect to nuclear coordinates: Complete formulation for electrostatic continuum solvation models. Journal of Chemical Physics, 1999, 110, 6858-6870. | 1.2 | 115 |
| 608 | Enthalpic anomeric effect in 2-Y-1,3-dithianes (Y = SC6H5, CO2CH2CH3, and COC6H5). Experimental and theoretical evaluation. Solvent effects. Tetrahedron, 1999, 55, 359-372. | 1.0 | 17 |
| 609 | Formation, characterization, and some reactions of spiro[cyclobutane-1,1 ^ˆ 2-1 ^ˆ 2H-azulenium] ion. Tetrahedron, 1999, 55, 12479-12492. | 1.0 | 4 |
| 610 | Molecular and vibrational structure of anthralin. Infrared linear dichroism spectroscopy and quantum chemical calculations. Journal of Molecular Structure, 1999, 475, 131-140. | 1.8 | 10 |
| 611 | An ab initio and matrix isolation infrared study of the 1:1 C2H2 ^ˆ CHCl3 adduct. Journal of Molecular Structure, 1999, 510, 59-68. | 1.8 | 50 |
| 612 | The electronic spectra of CaN+2 and Ca(N2)+2. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 457-466. | 2.0 | 5 |
| 613 | A fully ab initio quartic force field of spectroscopic quality for SO3. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 709-718. | 2.0 | 31 |
| 614 | Hyperfine parameters of pyridyl-containing iminoxy radicals generated from oximes by ^ˆ irradiation and in zeolite lattice: EPR spectroscopy and density functional study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 1699-1709. | 2.0 | 10 |
| 615 | A DFT study of the geometries and vibrational spectra of indene and some of its heterocyclic analogues, benzofuran, benzoxazole, bensothiophene, benzothiazole, indole and indazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 2437-2446. | 2.0 | 50 |
| 616 | The [Re, O8]+ potential energy surface: fourier transform ion cyclotron resonance collision induced dissociation studies and density functional calculations. International Journal of Mass Spectrometry, 1999, 185-187, 625-638. | 0.7 | 11 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 617 | Structure and stability of the CF ₃ ²⁺ dication. <i>International Journal of Mass Spectrometry</i> , 1999, 185-187, 701-706. | 0.7 | 14 |
| 618 | Acetylacetonate (acac) anion in the gas phase: predicted structures, vibrational spectra, and photodetachment energies. <i>International Journal of Mass Spectrometry</i> , 1999, 185-187, 577-587. | 0.7 | 6 |
| 619 | Pyrazine diradicals, carbenes, ylides, and distonic ions probed by theory and experiment. <i>International Journal of Mass Spectrometry</i> , 1999, 185-187, 925-933. | 0.7 | 22 |
| 620 | Experimental and theoretical studies of the basicity and proton affinity of SiF ₄ and the structure of SiF ₄ H ⁺ . <i>Journal of the American Society for Mass Spectrometry</i> , 1999, 10, 848-855. | 1.2 | 5 |
| 621 | Vibrational circular dichroism, absolute configuration and predominant conformations of volatile anesthetics: 1,2,2,2-tetrafluoroethyl methyl ether. <i>Tetrahedron: Asymmetry</i> , 1999, 10, 1099-1106. | 1.8 | 18 |
| 622 | Chiroptical properties of 12,15-dichloro[3.0]orthometacyclophane—correlations between molecular structure and circular dichroism spectra of a biphenylophane. <i>Tetrahedron: Asymmetry</i> , 1999, 10, 2153-2164. | 1.8 | 9 |
| 623 | Theoretical studies of pentene cracking on zeolites: C—C $\hat{\nu}$ -scission processes. <i>Catalysis Today</i> , 1999, 50, 517-523. | 2.2 | 42 |
| 624 | Theoretical study of the CH ₂ Br, CHBr ₂ and CBr ₃ radicals. <i>Chemical Physics</i> , 1999, 247, 365-373. | 0.9 | 10 |
| 625 | The atomization energy of Mg ₄ . <i>Chemical Physics Letters</i> , 1999, 300, 364-368. | 1.2 | 24 |
| 626 | On the performance of density functional theory for symmetry-breaking problems. <i>Chemical Physics Letters</i> , 1999, 302, 425-430. | 1.2 | 128 |
| 627 | Density functional calculations of the hyperpolarisabilities of small molecules. <i>Chemical Physics Letters</i> , 1999, 303, 391-398. | 1.2 | 46 |
| 628 | Structure and internal rotation in quadruply bonded $\hat{\nu}$ -Mo ₂ Cl ₄ (P—P) ₂ complexes: a density functional theory study of the cis-Mo ₂ Cl ₄ (PH ₃) ₄ complex. <i>Chemical Physics Letters</i> , 1999, 303, 621-628. | 1.2 | 11 |
| 629 | Gas-phase reactions of protonated chlorine, Cl ₂ H ⁺ , with H ₂ (D ₂) and CH ₄ . A mass spectrometric and theoretical study. <i>Chemical Physics Letters</i> , 1999, 304, 191-196. | 1.2 | 10 |
| 630 | DFT study on structures and vibrational frequencies of (CS ₂) ₂ ⁺ . <i>Chemical Physics Letters</i> , 1999, 304, 265-270. | 1.2 | 15 |
| 631 | The conformation and internal rotational barrier of benzyl fluoride. <i>Chemical Physics Letters</i> , 1999, 308, 160-164. | 1.2 | 16 |
| 632 | Basis set superposition error in atomic cluster calculations. <i>Chemical Physics Letters</i> , 1999, 314, 108-113. | 1.2 | 16 |
| 633 | Gaussian-3 theory using coupled cluster energies. <i>Chemical Physics Letters</i> , 1999, 314, 101-107. | 1.2 | 217 |
| 634 | Accurate D ₀ value for NF ⁺ . <i>Chemical Physics Letters</i> , 1999, 300, 80-84. | 1.2 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 635 | On the ground-state structure of XBO (X=Li, Na and K) molecules. <i>Chemical Physics Letters</i> , 1999, 301, 59-63. | 1.2 | 3 |
| 636 | Theoretical study of the quadrupole-bound anion (BeO) $2\hat{a}^-$. <i>Chemical Physics Letters</i> , 1999, 303, 65-75. | 1.2 | 23 |
| 637 | Theoretical study of the C3Cl radical and its cation. <i>Chemical Physics Letters</i> , 1999, 315, 224-232. | 1.2 | 18 |
| 638 | Chemical bonding and reactivity: a local thermodynamic viewpoint. <i>Chemical Physics Letters</i> , 1999, 314, 114-121. | 1.2 | 47 |
| 639 | The heat of formation of C2F4. <i>Chemical Physics Letters</i> , 1999, 315, 449-453. | 1.2 | 15 |
| 640 | HCN Synthesis from Methane and Ammonia: \hat{A} Mechanisms of Pt+-Mediated C \hat{a} -N Coupling. <i>Journal of the American Chemical Society</i> , 1999, 121, 10614-10625. | 6.6 | 116 |
| 641 | A new ONIOM implementation in Gaussian98. Part I. The calculation of energies, gradients, vibrational frequencies and electric field derivatives. <i>Computational and Theoretical Chemistry</i> , 1999, 461-462, 1-21. | 1.5 | 1,795 |
| 642 | DTMM and COSMIC molecular mechanics parameters for alkylsilanes. <i>Computational and Theoretical Chemistry</i> , 1999, 490, 219-232. | 1.5 | 4 |
| 644 | An ab initio study of the structures and properties of the XH42+ and XH62+ (X=C, Si, Ge) dications. <i>International Journal of Quantum Chemistry</i> , 1999, 72, 319-324. | 1.0 | 6 |
| 645 | New aspects of H2 activation by nickel-iron hydrogenase. <i>International Journal of Quantum Chemistry</i> , 1999, 73, 197-207. | 1.0 | 56 |
| 646 | Favorable performance of the DFT methods in predicting the minimum-energy structure of the lowest triplet state of WF4. <i>International Journal of Quantum Chemistry</i> , 1999, 73, 369-375. | 1.0 | 2 |
| 647 | Thermolysis mechanism of N-acetylpropanamide. <i>International Journal of Quantum Chemistry</i> , 1999, 74, 337-342. | 1.0 | 1 |
| 648 | Method for the evaluation of normal modes and molecular mechanics with reduced sets of force constants. 1. Principles and reliability test. <i>Journal of Raman Spectroscopy</i> , 1999, 30, 3-28. | 1.2 | 15 |
| 649 | Determination of force fields for nucleic acid bases. use of the ultraviolet resonance Raman intensities to check the vibrational assignments. <i>Journal of Raman Spectroscopy</i> , 1999, 30, 1001-1007. | 1.2 | 13 |
| 650 | Excitation energies of benzene from Kohn-Sham theory. , 1999, 20, 106-113. | | 77 |
| 651 | Compatibility of correlation-consistent basis sets with a hybrid Hartree-Fock/density functional method. <i>Journal of Computational Chemistry</i> , 1999, 20, 207-216. | 1.5 | 37 |
| 652 | Structural and Energetical Characterization of the Methylbutadiene \hat{a} -Fe(CO)3 Isomers and Related Reactive Intermediates with Quantum Chemical Methods. <i>European Journal of Inorganic Chemistry</i> , 1999, 1999, 1869-1880. | 1.0 | 15 |
| 653 | Substituent Effects on the Vinylcyclopropane \hat{a} -Cyclopentene Rearrangement \hat{a} - A Theoretical Study by Restricted and Unrestricted Density Functional Theory. <i>European Journal of Organic Chemistry</i> , 1999, 1999, 215-220. | 1.2 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 654 | [1,3]-Sigmatropic Rearrangements of Divinylcyclopropane Derivatives and Hetero Analogs in Competition with Cope-Type Rearrangements – A DFT Study. <i>European Journal of Organic Chemistry</i> , 1999, 1999, 1107-1114. | 1.2 | 22 |
| 655 | The Addition Patterns of C60 Trisadducts Involving the Positional Relationshipse andtrans-n (n = 2â€“4): Isolation, Properties, and Determination of the Absolute Configuration of Tris(malonates) and Tris[bis(oxazolines)]. , 1999, 1999, 3027-3039. | | 39 |
| 658 | Câˆ“H and Nâˆ“H Bond Dissociation Energies of Small Aromatic Hydrocarbons. <i>Journal of the American Chemical Society</i> , 1999, 121, 491-500. | 6.6 | 163 |
| 659 | On the Calculation and Modeling of Magnetic Exchange Interactions in Weakly Bonded Systems:Â The Case of the Ferromagnetic Copper(II) 1/42-Azido Bridged Complexes. <i>Inorganic Chemistry</i> , 1999, 38, 1996-2004. | 1.9 | 173 |
| 660 | The Different Nature of Bonding in Cu+-Glycine and Cu2+-Glycine. <i>Journal of Physical Chemistry B</i> , 1999, 103, 2310-2317. | 1.2 | 198 |
| 661 | Possibility of the Existence of Non-Carbon Fullerenes:â€% Ab Initio HF and DFT/B3LYP Studies of the IV Main Group Fullerene-Like Species. <i>Journal of Physical Chemistry A</i> , 1999, 103, 396-401. | 1.1 | 38 |
| 662 | Bond dissociation energies for substituted polycyclic aromatic hydrocarbons and their cations. <i>Molecular Physics</i> , 1999, 96, 471-476. | 0.8 | 31 |
| 663 | Density Functional Calculations of Hyperfine Coupling Constants in Alanine-Derived Radicals. <i>Journal of Physical Chemistry A</i> , 1999, 103, 6650-6657. | 1.1 | 42 |
| 664 | Calculation of dipole moment functions with density functional theory: application to vibrational band intensities. <i>Molecular Physics</i> , 1999, 96, 1125-1138. | 0.8 | 36 |
| 665 | Gas-Phase Ion Chemistry of Borazine, an Inorganic Analogue of Benzene. <i>Journal of the American Chemical Society</i> , 1999, 121, 11204-11210. | 6.6 | 63 |
| 666 | Methylsulfonyl and Methoxysulfinyl Radicals and Cations in the Gas Phase. A Variable-Time and Photoexcitation Neutralizationâˆ“Reionization Mass Spectrometric and ab Initio/RRKM Study. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5348-5361. | 1.1 | 44 |
| 667 | Experimental and ab initio spectra of the persistent carbocation generated upon adsorption of vinylanisole in acid zeolites. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 3689-3695. | 1.3 | 15 |
| 668 | Flowing afterglow study of the gas phase nucleophilic reactions of some formyl, acetyl and cyclic esters. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 2397-2407. | 0.9 | 16 |
| 669 | Coumarin 153 in the gas phase: optical spectra and quantum chemical calculations. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 3209-3218. | 1.3 | 94 |
| 670 | An analysis of chlorine and bromine oxygen bonding and its implications for stratospheric chemistry. <i>Molecular Physics</i> , 1999, 96, 633-643. | 0.8 | 25 |
| 671 | Ion association of alkali and alkaline earth metal azides in dimethylsulfoxide. Infrared spectrometry and ab initio calculations. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 4701-4706. | 1.3 | 23 |
| 672 | Structure and low-frequency vibrational properties of (H2O)10 composed of a ring form of (H2O)4 and a cage form of (H2O)6. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 3473-3479. | 1.3 | 2 |
| 673 | Glycine radicals in the gas phaseâ€“â€“. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 2315-2323. | 0.9 | 43 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 674 | Geometry and electronic structure of bis-(glycinato)-CuII·2H2O complexes as studied by density functional B3LYP computations. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 4157-4163. | 1.3 | 44 |
| 675 | Determination of absolute configuration using circular dichroism: Tröger's Base revisited using vibrational circular dichroism. <i>Chemical Communications</i> , 1999, , 361-362. | 2.2 | 32 |
| 676 | Experimental and theoretical studies of a chiral azulenophane: synthesis, structure and circular dichroism spectra of 14,17-dimethyl[2](1,3)azuleno[2]paracyclophane. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 521-528. | 0.9 | 11 |
| 677 | An Active Site Model and the Catalytic Activity Mechanism of the new Fullerene-Based Catalyst - (I ²⁺ -C ₆₀)Pd(PPh ₃) ₂ . <i>Fullerenes, Nanotubes, and Carbon Nanostructures</i> , 1999, 7, 467-484. | 0.6 | 9 |
| 678 | A quantum mechanical periodic ab initio approach to materials science: the CRYSTAL program. <i>Solid State Sciences</i> , 1999, 1, 147-155. | 0.8 | 8 |
| 679 | Gaussian-3 theory using density functional geometries and zero-point energies. <i>Journal of Chemical Physics</i> , 1999, 110, 7650-7657. | 1.2 | 1,606 |
| 680 | Ab initio cluster model approach to the chemisorption of NH ₃ on Pt(111). <i>Surface Science</i> , 1999, 430, 18-28. | 0.8 | 44 |
| 681 | Hydrogen abstraction from a diamond(111) surface in a uniform electric field. <i>Surface Science</i> , 1999, 429, 199-205. | 0.8 | 6 |
| 682 | Theoretical study of the Cl-passivated Si(111) surface. <i>Surface Science</i> , 1999, 430, 116-125. | 0.8 | 13 |
| 683 | Theoretical studies of H ₂ desorption processes in chemical vapor deposition of boron-doped silicon surfaces. <i>Surface Science</i> , 1999, 436, 175-192. | 0.8 | 11 |
| 684 | Gas-Phase Thermochemistry of Iron Oxides and Hydroxides: a Portrait of a Super-Efficient Flame Suppressant. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1150-1159. | 1.1 | 52 |
| 685 | Electronic Structure and Properties of FeO and FeO-Clusters. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5812-5822. | 1.1 | 72 |
| 686 | A density functional study of lithium bulk and surfaces. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 5007-5019. | 0.7 | 74 |
| 687 | A Further Study of the Products of Scandium and Dioxygen Reactions. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5463-5467. | 1.1 | 59 |
| 688 | DENSITYFUNCTIONALTHEORY OFBIOLOGICALLYRELEVANTMETALCENTERS. <i>Annual Review of Physical Chemistry</i> , 1999, 50, 221-249. | 4.8 | 250 |
| 689 | Heats of Formation for PO and POH (n = 1-3). <i>Journal of Physical Chemistry A</i> , 1999, 103, 11126-11129. | 1.1 | 22 |
| 690 | A complete basis set model chemistry. VI. Use of density functional geometries and frequencies. <i>Journal of Chemical Physics</i> , 1999, 110, 2822-2827. | 1.2 | 2,451 |
| 691 | The [C ₆ H ₁₀] ⁺ Hypersurface: the Parent Radical Cation Diels-Alder Reaction. <i>Journal of the American Chemical Society</i> , 1999, 121, 6719-6729. | 6.6 | 37 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 692 | A Quantum Chemical Study of the Mechanism of Tyrosinase. <i>Journal of Physical Chemistry B</i> , 1999, 103, 1193-1202. | 1.2 | 71 |
| 693 | Molecular Structure in Solution: An ab Initio Vibrational Spectroscopy Study of Phenyloxirane. <i>Journal of the American Chemical Society</i> , 1999, 121, 2836-2849. | 6.6 | 40 |
| 694 | A Hard-Soft Acid-Base and DFT Analysis of Singlet-Triplet Gaps and the Addition of Singlet Carbenes to Alkenes. <i>Journal of Organic Chemistry</i> , 1999, 64, 7061-7066. | 1.7 | 94 |
| 695 | Oxidative Aromatic Substitutions: Hartree-Fock/Density Functional and ab Initio Molecular Orbital Studies of Benzene and Toluene Nitrosation. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4261-4269. | 1.1 | 42 |
| 696 | Nature of the Metal-Alkene Bond in Platinum Complexes of Strained Olefins. <i>Organometallics</i> , 1999, 18, 457-465. | 1.1 | 59 |
| 697 | Density Functional Theory Investigation of the Electronic Structure and Spin Density Distribution in Peroxyl Radicals. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1619-1626. | 1.1 | 30 |
| 698 | Pathways for the Reaction of the Butadiene Radical Cation, $[C_4H_6]^{\bullet+}$, with Ethylene. <i>Journal of Physical Chemistry A</i> , 1999, 103, 8895-8905. | 1.1 | 25 |
| 699 | DFT Study of the Role of Bridging Diphosphine Ligands in the Structure and the Internal Rotation in Quadruply Bonded Metal Dimers of the $Mo_2Cl_4(P)_2$ Type. <i>Inorganic Chemistry</i> , 1999, 38, 5443-5448. | 1.9 | 14 |
| 700 | Ab Initio Density Functional Theory Study of the Structure and Vibrational Spectra of Cyclohexanone and its Isotopomers. <i>Journal of Physical Chemistry A</i> , 1999, 103, 527-538. | 1.1 | 34 |
| 701 | Why Does the Reaction of the Dihydrogen Molecule with $[P_2N_2]Zr(\eta^4-\eta^2-N_2)Zr[P_2N_2]$ Produce $[P_2N_2]Zr(\eta^4-\eta^2-N_2H)Zr[P_2N_2](\eta^4-H)$ but Not the Thermodynamically More Favorable $[P_2N_2]Zr(\eta^4-NH)Zr[P_2N_2]$? A Theoretical Study. <i>Journal of the American Chemical Society</i> , 1999, 121, 5754-5761. | | 41 |
| 702 | Influence of Electrostatic Effects on Activation Barriers in Enzymatic Reactions: A Pyridoxal 5'-Phosphate-Dependent Decarboxylation of α -Amino Acids. <i>Journal of the American Chemical Society</i> , 1999, 121, 6542-6555. | 6.6 | 66 |
| 703 | Hyperconjugative Effects in Carbenium and Silicenium Ions. <i>Journal of Physical Chemistry A</i> , 1999, 103, 6458-6467. | 1.1 | 19 |
| 704 | Direct Dynamics for Free Radical Kinetics in Solution: A Solvent Effect on the Rate Constant for the Reaction of Methanol with Atomic Hydrogen. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4893-4909. | 1.1 | 103 |
| 705 | Dimer Cations of Cyanoacetylene: A Theoretical Isomers and Their Laboratory Production in the Absence and Presence of $C_6O_2^+$. Implications for Interstellar/Circumstellar Chemistry. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7528-7534. | 1.1 | 21 |
| 706 | Theoretical Study on the Origin of Enantioselectivity in the Bis(dihydroquinidine)-3,6-pyridazine-Osmium Tetroxide-Catalyzed Dihydroxylation of Styrene. <i>Journal of the American Chemical Society</i> , 1999, 121, 1317-1323. | 6.6 | 94 |
| 707 | The d ₀ , d ₁ and d ₂ Configurations in Known and Unknown Tetrathiometal Compounds MS_4n (M = Mo, Tc, U) T_j $ETQq_{1,1,0.7843,1.4}rgBT_{23}$ | 1.9 | 23 |
| 708 | Hydrogen Atom or Proton Transfer in Neutral and Single Positive Ions of Salicylic Acid and Related Compounds. <i>Journal of the American Chemical Society</i> , 1999, 121, 8882-8890. | 6.6 | 48 |
| 709 | A Quantum-Chemical Study of the $C_2H_3F_2^+$ and $C_2H_3Cl_2^+$ Isomers and Their Interconversion. CBS-QB3 Proton Affinities of Difluoroethenes and Dichloroethenes. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7872-7882. | 1.1 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 710 | (Hydroxyalkyl)pyridinooxazolines in Palladium-Catalyzed Allylic Substitutions. Conformational Preferences of the Ligand. <i>Organometallics</i> , 1999, 18, 4900-4907. | 1.1 | 22 |
| 711 | Laser Flash Photolysis and Computational Study of Singlet Phenylnitrene. <i>Journal of the American Chemical Society</i> , 1999, 121, 1202-1207. | 6.6 | 121 |
| 712 | NMR Chemical Shifts. 2. Interpretation of the Carbon Chemical Shifts in Monocyclic Aromatic Compounds and Carbenes. <i>Journal of Physical Chemistry A</i> , 1999, 103, 21-27. | 1.1 | 32 |
| 713 | A Coupled-Cluster Analysis of the Electronic Excited States in Aminobenzonitriles. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4056-4064. | 1.1 | 54 |
| 714 | Timing Is Critical: Effect of Spin Changes on the Diastereoselectivity in Mn(salen)-Catalyzed Epoxidation. <i>Journal of the American Chemical Society</i> , 1999, 121, 5083-5084. | 6.6 | 119 |
| 715 | A DFT/Electron Localization Function (ELF) Study of the Bonding of Phosphinidenes with N-Heterocyclic Carbenes. <i>Journal of Physical Chemistry A</i> , 1999, 103, 10998-11003. | 1.1 | 48 |
| 716 | Theoretical C-H Bond Dissociation Enthalpies for CH ₃ Br and CH ₂ ClBr. <i>Journal of Physical Chemistry A</i> , 1999, 103, 6387-6393. | 1.1 | 17 |
| 717 | Mechanism of Hydroxyl Radical Addition to Imidazole and Subsequent Water Elimination. <i>Journal of Physical Chemistry B</i> , 1999, 103, 5598-5607. | 1.2 | 33 |
| 718 | Accurate Heats of Formation for BF _n , BF _n ⁺ , BCl _n , and BCl _n ⁺ for n = 1-3. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4313-4318. | 1.1 | 30 |
| 719 | Ab initio Studies of NH ₄ ⁺ (H ₂ O) ₁₋₅ and the Influence of Hydrogen-Bonding Nonadditivity on Geometries and Vibrations. <i>Journal of Physical Chemistry A</i> , 1999, 103, 3123-3135. | 1.1 | 64 |
| 720 | Density Functional Calculation of ¹ J _{C-H} Coupling Constants in Cyclohexane and Diheterocyclohexanes. Repercussion of Stereoelectronic Effects on Coupling Constants. <i>Journal of Physical Chemistry A</i> , 1999, 103, 932-937. | 1.1 | 68 |
| 721 | Evidence for Sulfur-Based Radicals in Thiolate Compound I Intermediates. <i>Journal of the American Chemical Society</i> , 1999, 121, 7939-7940. | 6.6 | 195 |
| 722 | Generation of Two Isomers of C ₅ H from the Corresponding Anions. A Theoretically Motivated Mass Spectrometric Study. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5161-5170. | 1.1 | 39 |
| 723 | Quantum Chemical Studies on the Thermochemistry of Alkyl and Peroxyl Radicals. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7094-7104. | 1.1 | 65 |
| 724 | Modeling Nucleobase Radicals in the Gas Phase. Experimental and Computational Study of 2-Hydroxypyridinium and 2-(1H)Pyridone Radicals. <i>Journal of Physical Chemistry A</i> , 1999, 103, 6268-6281. | 1.1 | 53 |
| 725 | Glycyl Radical Is a Stable Species in the Gas Phase. <i>Journal of the American Chemical Society</i> , 1999, 121, 7955-7956. | 6.6 | 45 |
| 726 | Hydrogen Atom Addition to Hydrocarbon Guests in Radiolyzed Zeolites. <i>Journal of Physical Chemistry B</i> , 1999, 103, 9219-9230. | 1.2 | 25 |
| 727 | Potential Energy Function and Vibrational States of the Electronic Ground State of N ₄ ⁺ . <i>Journal of Physical Chemistry A</i> , 1999, 103, 1846-1852. | 1.1 | 37 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 728 | Propyne Pyrolysis in a Flow Reactor: An Experimental, RRKM, and Detailed Kinetic Modeling Study. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5889-5899. | 1.1 | 116 |
| 729 | Synthesis and Characterization of OsH ₂ Cl[¹⁵ N, ¹⁸ O-(ONCR ₂)](PiPr ₃) ₂ (CR ₂ = C(CH ₂) ₄ CH ₂ , R = CH ₃): Influence of the L ₂ Ligand on the Nature of the H ₂ Unit in OsH ₂ ClL ₂ (PiPr ₃) ₂ (L ₂ = ONCR ₂ , NHC(Ph)C ₆ H ₄) Complexes. <i>Organometallics</i> , 1999, 18, 4296-4303. | 1.1 | 17 |
| 730 | Interconversion of FeC ₂ H ₃ ⁺ and HFeC ₂ H ₂ ⁺ : An FTICR and Density Functional Study. <i>Organometallics</i> , 1999, 18, 5460-5469. | 1.1 | 4 |
| 731 | Coupling Trans-Bent Double Bonds in Tetragermabutadiene. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4723-4736. | 1.1 | 8 |
| 732 | Theoretical Model Studies of the Iron Dimer Complex of MMO and RNR. <i>Inorganic Chemistry</i> , 1999, 38, 2880-2889. | 1.9 | 144 |
| 733 | Dissociation Energies and Kinetics of Aminopyrimidinium Radicals by ab Initio and Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1905-1912. | 1.1 | 35 |
| 734 | A Hybrid Density Functional Theory/Molecular Mechanics Study of Nickel-Iron Hydrogenase: Investigation of the Active Site Redox States. <i>Journal of the American Chemical Society</i> , 1999, 121, 4468-4477. | 6.6 | 142 |
| 735 | Gas-Phase Generation and Photoelectron Spectra of Dimethyl- and Diisopropylsilanethiones. <i>Organometallics</i> , 1999, 18, 4795-4799. | 1.1 | 6 |
| 736 | Generation, Characterization, and Reactivity of the Transition Metal-ortho-Benzyne Analog of Pyrazine (Fe- ^{2,3} -Didehydropyrazine) in the Gas Phase: An Experimental and Theoretical Study. <i>Organometallics</i> , 1999, 18, 1774-1785. | 1.1 | 9 |
| 737 | Conformational Analysis Using ab Initio Vibrational Spectroscopy: 3-Methylcyclohexanone. <i>Journal of the American Chemical Society</i> , 1999, 121, 7413-7414. | 6.6 | 58 |
| 738 | Water Exchange Reactions and Hydrolysis of Hydrated Titanium(III) Ions. A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9899-9905. | 1.1 | 57 |
| 739 | Theoretical Predictions and Single-Crystal Neutron Diffraction and Inelastic Neutron Scattering Studies on the Reaction of Dihydrogen with the Dinuclear Dinitrogen Complex of Zirconium [P ₂ N ₂]Zr(^{1,4-η-2-N₂)Zr[P₂N₂], P₂N₂= PhP(CH₂SiMe₂NSiMe₂CH₂)₂PPh. <i>Journal of the American Chemical Society</i>, 1999, 121, 523-528.} | 6.6 | 106 |
| 740 | Reaction Mechanism of Compound I Formation in Heme Peroxidases: A Density Functional Theory Study. <i>Journal of the American Chemical Society</i> , 1999, 121, 10178-10185. | 6.6 | 132 |
| 741 | Thermally Activated Site Exchange and Quantum Exchange Coupling Processes in Unsymmetrical Trihydride Osmium Compounds. <i>Inorganic Chemistry</i> , 1999, 38, 1814-1824. | 1.9 | 38 |
| 742 | Heats of Formation for CF _n (n= 1-4), CF _n ⁺ (n= 1-4), and CF _n ⁻ (n=1-3). <i>Journal of Physical Chemistry A</i> , 1999, 103, 1876-1879. | 1.1 | 20 |
| 743 | Accurate Indium Bond Energies. <i>Journal of Physical Chemistry A</i> , 1999, 103, 6429-6432. | 1.1 | 21 |
| 744 | Tetradehydrobenzenes: Singlet-Triplet Energy Separations and Vibrational Frequencies. <i>Journal of the American Chemical Society</i> , 1999, 121, 2829-2835. | 6.6 | 44 |
| 745 | An Experimental and Theoretical Study of the Substituent Effects on the Redox Properties of 2-[(R-phenyl)amine]-1,4-naphthalenediones in Acetonitrile. <i>Journal of Organic Chemistry</i> , 1999, 64, 3684-3694. | 1.7 | 99 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 746 | Vibrational Circular Dichroism, Absolute Configuration, and Predominant Conformations of Volatile Anesthetics: Desflurane. <i>Journal of Physical Chemistry B</i> , 1999, 103, 6127-6132. | 1.2 | 30 |
| 747 | Gaseous Trihalogen Cations. Formation, Structure and Reactivity of Cl ₃ ⁺ and Cl ₂ F ⁺ Ions from a Joint ab Initio and FT-ICR Study. <i>Journal of Physical Chemistry A</i> , 1999, 103, 2128-2133. | 1.1 | 10 |
| 748 | Heterocyclic Radicals in the Gas Phase. An Experimental and Computational Study of 3-Hydroxypyridinium Radicals and Cations. <i>Journal of the American Chemical Society</i> , 1999, 121, 6010-6018. | 6.6 | 49 |
| 749 | Ultrafast Infrared Studies of the Reaction Mechanism of Silicon-Hydrogen Bond Activation by δ -5-CpV(CO) ₄ . <i>Journal of Physical Chemistry A</i> , 1999, 103, 10426-10432. | 1.1 | 34 |
| 750 | Theory as a viable partner for experiment—The quest for trivalent silylium ions in solution. <i>Theoretical and Computational Chemistry</i> , 1999, 6, 231-301. | 0.2 | 6 |
| 751 | Theoretical and Experimental Studies of the Benzene Radical Cation: Effects of Selective Deuteration. <i>Advances in Quantum Chemistry</i> , 1999, 35, 339-355. | 0.4 | 4 |
| 752 | Density functional computations and mass spectrometric measurements. Can this coupling enlarge the knowledge of gas-phase chemistry?. <i>Advances in Quantum Chemistry</i> , 2000, 36, 93-120. | 0.4 | 16 |
| 753 | Autoionization-Detected Infrared Spectroscopy of Jet-Cooled Naphthol Cations. <i>Journal of Physical Chemistry A</i> , 2000, 104, 7227-7232. | 1.1 | 20 |
| 754 | Direct Study on the Unimolecular Decomposition of Methoxy Radicals: The Role of the Tunneling Effect. <i>Bulletin of the Chemical Society of Japan</i> , 2000, 73, 53-60. | 2.0 | 16 |
| 755 | Potential interstellar molecules. Formation of neutral C ₆ CO from C ₆ CO ⁺ in the gas phase. , 2000, 14, 118-121. | | 8 |
| 756 | Simulations of oligopeptide vibrational CD: Effects of isotopic labeling. <i>Biopolymers</i> , 2000, 53, 380-395. | 1.2 | 73 |
| 757 | Intermolecular hydrogen abstraction from triplet excited state of decafluorobenzophenone: a Raman investigation. <i>Journal of Raman Spectroscopy</i> , 2000, 31, 331-338. | 1.2 | 13 |
| 758 | Theoretical modeling of the heme group with a hybrid QM/MM method. <i>Journal of Computational Chemistry</i> , 2000, 21, 282-294. | 1.5 | 39 |
| 759 | A comparative study of DFT and traditional ab initio methodologies on the OsO ₄ molecule. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 544-551. | 1.0 | 9 |
| 760 | CRYSTAL and EMBED, two computational tools for the ab initio study of electronic properties of crystals. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 1032-1048. | 1.0 | 46 |
| 761 | Quantum chemical calculation of Henry constants of diatomic molecules in faujasite-type zeolites. <i>Journal of Computational Chemistry</i> , 2000, 21, 909-922. | 1.5 | 20 |
| 762 | Proton affinity of peroxyacetyl nitrate. A computational study of topical proton affinities. <i>Journal of Mass Spectrometry</i> , 2000, 35, 1351-1359. | 0.7 | 9 |
| 763 | Infrared and Raman spectra of a new radical cation charged defect created on a well-barrier-well thiophene-based oligomer. <i>Journal of Raman Spectroscopy</i> , 2000, 31, 565-570. | 1.2 | 23 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 764 | Calculations and electron spin resonance spectra of syringic and sinapinic acid. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 1210-1215. | 1.0 | 1 |
| 769 | Vibrational Circular Dichroism and Absolute Configuration of Chiral Sulfoxides: <i>tert</i> -Butyl Methyl Sulfoxide. <i>Chemistry - A European Journal</i> , 2000, 6, 4479-4486. | 1.7 | 44 |
| 770 | 4-Oxo-2,3,5,6-tetrafluorocyclohexa-2,5-dienylideneâ€”A Highly Electrophilic Triplet Carbene. <i>Chemistry - A European Journal</i> , 2000, 6, 4567-4579. | 1.7 | 43 |
| 771 | The High-Valent Compound of Cytochrome P450: The Nature of the Feâ€”S Bond and the Role of the Thiolate Ligand as an Internal Electron Donor. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 3851-3855. | 7.2 | 97 |
| 772 | Câ€”H Activation by Direct Boraneâ€”Hydrocarbon Dehydrogenation: Kinetic and Thermodynamic Aspects. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 4136-4139. | 7.2 | 37 |
| 773 | Why Static Molecular Parameters Cannot Characterize the Free Radical Scavenging Activity of Phenolic Antioxidants. <i>QSAR and Combinatorial Science</i> , 2000, 19, 375-379. | 1.4 | 23 |
| 774 | Alkane Hydroxylation by Cytochrome P450: Is Kinetic Isotope Effect a Reliable Probe of Transition State Structure?. <i>European Journal of Inorganic Chemistry</i> , 2000, 2000, 2455-2458. | 1.0 | 35 |
| 775 | 1,2,3,4-Tetra- <i>tert</i> -butyl-4-trimethylsilyl-4-sila-2-cyclobuten-1-yl: A Quantum Mechanical and ESR Study. <i>European Journal of Organic Chemistry</i> , 2000, 2000, 1107-1112. | 1.2 | 9 |
| 776 | A quantum mechanical study of the ionic interactions in model compounds of polyelectrolyteâ€”surfactant complexes derived from polypeptides. <i>Chemical Physics Letters</i> , 2000, 319, 318-326. | 1.2 | 17 |
| 777 | Hybrid density functional approach to the structures and EPR parameters of $\dot{\text{I}}\text{f}$ -type iminoxy radicals: the case of 3-oxobutan-2-iminoxy. <i>Chemical Physics Letters</i> , 2000, 319, 611-617. | 1.2 | 21 |
| 778 | Hydrogen and fluorine binding to the sidewalls of a (10,0) carbon nanotube. <i>Chemical Physics Letters</i> , 2000, 322, 237-241. | 1.2 | 134 |
| 779 | Heats of formation for ClFn ($n=1\text{â€”}3$). <i>Chemical Physics Letters</i> , 2000, 323, 498-505. | 1.2 | 9 |
| 780 | Mechanisms for polycyclic aromatic hydrocarbon (PAH) growth. <i>Chemical Physics Letters</i> , 2000, 326, 283-287. | 1.2 | 69 |
| 781 | Static and dynamic polarisabilities, Cauchy coefficients and their anisotropies: an evaluation of DFT functionals. <i>Chemical Physics Letters</i> , 2000, 328, 446-452. | 1.2 | 38 |
| 782 | Artificial symmetry breaking in radicals is avoided by the use of the Ensemble-Referenced Kohnâ€”Sham (REKS) method. <i>Chemical Physics Letters</i> , 2000, 332, 409-419. | 1.2 | 24 |
| 783 | Assessment of exchange correlation functionals. <i>Chemical Physics Letters</i> , 2000, 316, 160-166. | 1.2 | 104 |
| 784 | Geometric derivatives of density functional theory excitation energies using gradient-corrected functionals. <i>Chemical Physics Letters</i> , 2000, 317, 159-164. | 1.2 | 330 |
| 785 | Structural preferences of quadruply bonded bimetallic complexes. A DFT study of the chelated ($\dot{\text{I}}_{\pm}$) and bridged ($\dot{\text{I}}_2$) isomers in Mo ₂ Cl ₄ (H ₂ P(CH ₂) _n PH ₂) ₂ ($n=1, 2$). <i>Inorganica Chimica Acta</i> , 2000, 300-302, 837-845. | 1.2 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 786 | Vibrational circular dichroism, absolute configuration and predominant conformations of volatile anesthetics: enflurane. <i>Journal of Molecular Structure</i> , 2000, 550-551, 105-115. | 1.8 | 18 |
| 787 | Medium effects on the ionization of the acidic sites of bifunctional organic molecules: the case of 4-hydroxybenzoic acid. <i>Journal of Molecular Structure</i> , 2000, 556, 245-252. | 1.8 | 8 |
| 788 | Tetracyclo[3.1.0.0(1.3).0(3.5)]hexane: a new C ₆ H ₆ isomer with an unusual bonding situation. <i>Journal of Molecular Structure</i> , 2000, 556, 23-32. | 1.8 | 6 |
| 789 | Calculated heats of formation of simple phosphinidenes (phosphanylidenes, R ² P). <i>Journal of Molecular Structure</i> , 2000, 556, 143-149. | 1.8 | 10 |
| 790 | Density functional study on the structures and vibrational spectra of the radical cation and dication of 1,1'-bis(aminomethyl)quaterthiophene. <i>Journal of Molecular Structure</i> , 2000, 521, 249-260. | 1.8 | 6 |
| 791 | Formation and characterization of cyclic and polycyclic silthianes containing Si-Si bonds. <i>Journal of Organometallic Chemistry</i> , 2000, 602, 193-207. | 0.8 | 34 |
| 792 | Synthesis, Stability, and X-Ray Crystallographic Structure Analysis of Spiro[1H-azulenium-1,1'-cycloalkane] Ions. <i>Tetrahedron</i> , 2000, 56, 9917-9925. | 1.0 | 22 |
| 793 | Spin-forbidden F ⁺ transfer between 2NF ⁺ and CO: a computational study on the detailed mechanistic aspects. <i>International Journal of Mass Spectrometry</i> , 2000, 201, 151-160. | 0.7 | 3 |
| 794 | Electron-impact total ionization cross sections of SF _x (x = 1-5). <i>International Journal of Mass Spectrometry</i> , 2000, 201, 187-195. | 0.7 | 44 |
| 795 | Structural and electronic characterisation of the organometallic distonic ion (C ₆ H ₆)Fe ⁺ (p-C ₆ H ₄) ⁻ . <i>International Journal of Mass Spectrometry</i> , 2000, 201, 297-305. | 0.7 | 7 |
| 796 | A mass spectrometric and computational study of gaseous peroxyxynitric acid and (HOONO ₂)H ⁺ protomers. <i>International Journal of Mass Spectrometry</i> , 2000, 195-196, 1-10. | 0.7 | 11 |
| 797 | High-energy [C ₃ H ₃ N ₂ O] cation radicals and molecules. <i>International Journal of Mass Spectrometry</i> , 2000, 195-196, 101-114. | 0.7 | 9 |
| 798 | Coordination chemistry of manganese-salen complexes studied by electrospray tandem mass spectrometry: the significance of axial ligands. <i>International Journal of Mass Spectrometry</i> , 2000, 195-196, 351-362. | 0.7 | 53 |
| 799 | Protonation sites in methyl nitrate and the formation of transient CH ₄ NO ₃ radicals. A neutralization-reionization mass spectrometric and computational study. <i>Journal of the American Society for Mass Spectrometry</i> , 2000, 11, 380-392. | 1.2 | 9 |
| 800 | Acyclic distonic acylium ions: Dual free radical and acylium ion reactivity in a single molecule. <i>Journal of the American Society for Mass Spectrometry</i> , 2000, 11, 697-704. | 1.2 | 19 |
| 801 | Proton affinity of uracil. A computational study of protonation sites. <i>Journal of the American Society for Mass Spectrometry</i> , 2000, 11, 1065-1071. | 1.2 | 74 |
| 802 | A theoretical exploratory study of low-energy (1-2 eV) electron catalysis in the gas phase process. <i>Chemical Physics</i> , 2000, 254, 99-108. | 0.9 | 4 |
| 803 | An experimental and theoretical study of the valence shell photoelectron spectrum of the chlorobenzene molecule. <i>Chemical Physics</i> , 2000, 254, 385-405. | 0.9 | 40 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 804 | Silylcyanides and silylisocyanides: a comparative theoretical study. <i>Chemical Physics</i> , 2000, 254, 187-202. | 0.9 | 8 |
| 805 | Structures, vibrational absorption and vibrational circular dichroism spectra of L-alanine in aqueous solution: a density functional theory and RHF study. <i>Chemical Physics</i> , 2000, 255, 165-194. | 0.9 | 84 |
| 806 | Theoretical study of structures, energetics and vibrational properties of BC ₂ H ₅ species. <i>Chemical Physics</i> , 2000, 255, 205-215. | 0.9 | 15 |
| 807 | The equilibrium N-H bond length. <i>Chemical Physics</i> , 2000, 260, 65-81. | 0.9 | 58 |
| 808 | Vibronic interactions in {6} and {18}hetero(A,B)annulenes. <i>Chemical Physics</i> , 2000, 260, 303-315. | 0.9 | 3 |
| 809 | An experimental and theoretical study of the valence shell photoelectron spectrum of bromobenzene. <i>Chemical Physics</i> , 2000, 252, 257-278. | 0.9 | 29 |
| 810 | Quantum mechanical calculations of molecular properties and ideal gas heat capacity of difluoromethane. <i>Fluid Phase Equilibria</i> , 2000, 170, 285-296. | 1.4 | 5 |
| 811 | O-O bond splitting mechanism in cytochrome oxidase. <i>Journal of Inorganic Biochemistry</i> , 2000, 80, 261-269. | 1.5 | 83 |
| 812 | Computational prediction of the ISC rate for triplet norbornene. <i>Chemical Physics Letters</i> , 2000, 322, 358-362. | 1.2 | 19 |
| 813 | Direct calculation of anharmonic vibrational states of polyatomic molecules using density functional theory: spectroscopic tests of recently developed functionals. <i>Chemical Physics Letters</i> , 2000, 324, 206-212. | 1.2 | 37 |
| 814 | The reactions of polycyclic aromatic hydrocarbons with OH. <i>Chemical Physics Letters</i> , 2000, 328, 396-402. | 1.2 | 32 |
| 815 | Infrared spectra of polycyclic aromatic hydrocarbons (PAHs). <i>Chemical Physics</i> , 2000, 262, 285-291. | 0.9 | 52 |
| 816 | Ab initio and equilibrium bond angles. Structures of HNO and H ₂ O ₂ . <i>Computational and Theoretical Chemistry</i> , 2000, 500, 245-258. | 1.5 | 31 |
| 817 | Performance and basis set dependence of density functional theory dipole and quadrupole moments. <i>Computational and Theoretical Chemistry</i> , 2000, 506, 1-8. | 1.5 | 31 |
| 818 | Structure and stability of enediynes containing heteroatoms—a quantum chemical investigation. <i>Computational and Theoretical Chemistry</i> , 2000, 506, 191-211. | 1.5 | 29 |
| 819 | The platinum-ethylene binding energy in Pt(PL ₃) ₂ (C ₂ H ₄). <i>Computational and Theoretical Chemistry</i> , 2000, 506, 223-232. | 1.5 | 21 |
| 820 | Insights from Coulomb and exchange intracules. <i>Computational and Theoretical Chemistry</i> , 2000, 506, 303-312. | 1.5 | 26 |
| 821 | Effects of hydration on the molecular structure of metal ion-atrazine dimer complexes: a MOPAC (PM3) study. <i>Computational and Theoretical Chemistry</i> , 2000, 531, 89-98. | 1.5 | 31 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 822 | DFT computational studies of intramolecular hydrogen-bonding interactions in a model system for 5-iminodaunomycin. <i>Computational and Theoretical Chemistry</i> , 2000, 529, 83-97. | 1.5 | 15 |
| 823 | An ab initio molecular orbital theory and density functional theory study of the conformational free energies of methyltetrahydro-2H-thiopyrans. <i>Computational and Theoretical Chemistry</i> , 2000, 529, 225-239. | 1.5 | 17 |
| 824 | A theoretical study of the molecular structure and vibrational spectra of methyl cyanate and its sulfur and selenium analogues. <i>Computational and Theoretical Chemistry</i> , 2000, 501-502, 277-284. | 1.5 | 6 |
| 825 | Density functional theory predictions for small radicals containing boron and aluminium: broken symmetry problems and solutions. <i>Molecular Physics</i> , 2000, 98, 961-966. | 0.8 | 6 |
| 826 | Structures, C-H and C-CH ₃ bond energies at borders of polycyclic aromatic hydrocarbons. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 5084-5088. | 1.3 | 48 |
| 827 | The preferred conformation of N- ¹⁵ -fluoroethylamides. Observation of the fluorine amide gauche effect. <i>Perkin Transactions II RSC</i> , 2000, , 605-607. | 1.1 | 60 |
| 828 | Using density functional theory for analysis of quadrupole coupling constants and Mössbauer isomer shifts of halogen compounds. <i>Journal of Structural Chemistry</i> , 2000, 41, 697-700. | 0.3 | 2 |
| 829 | EPR and density functional studies on 3-pyridylmethaniminoxy radical: ¹ H hyperfine couplings as a structural criterion for iminoxyls derived from pyridinealoximes. <i>Applied Magnetic Resonance</i> , 2000, 18, 85-100. | 0.6 | 13 |
| 830 | C ₃ -Symmetric Azaphosphatranes. <i>Collection of Czechoslovak Chemical Communications</i> , 2000, 65, 570-576. | 1.0 | 6 |
| 831 | A theoretical study of the reaction of Ti ⁺ with ethane. <i>Journal of Chemical Physics</i> , 2000, 112, 10247-10258. | 1.2 | 28 |
| 832 | Application of time-dependent density-functional theory to the 3 ¹ Σ ⁺ first excited state of H ₂ . <i>Journal of Chemical Physics</i> , 2000, 112, 527-530. | 1.2 | 52 |
| 833 | Infrared spectroscopy of CH stretching vibrations of jet-cooled alkylbenzene cations by using the "messenger" technique. <i>Journal of Chemical Physics</i> , 2000, 112, 6275-6284. | 1.2 | 68 |
| 834 | Resonant ion-dip infrared spectroscopy of benzene-(water) ₉ : Expanding the cube. <i>Journal of Chemical Physics</i> , 2000, 113, 2290-2303. | 1.2 | 81 |
| 835 | Solvation of magnesium and singly ionized magnesium atoms in NH ₃ clusters: Theory and experiment. <i>Journal of Chemical Physics</i> , 2000, 112, 10912-10925. | 1.2 | 29 |
| 836 | (MgO) _n ⁺ (n=1-5) Clusters: Multipole-Bound Anions and Photodetachment Spectroscopy. <i>Physical Review Letters</i> , 2000, 85, 3145-3148. | 2.9 | 51 |
| 837 | Structure and Formation Mechanism of Ge ²⁺ Center from Divalent Defects in Ge-doped SiO ₂ Glass. <i>Physical Review Letters</i> , 2000, 84, 1475-1478. | 2.9 | 40 |
| 838 | The reaction of benzene with a ground state carbon atom, C(3P _j). <i>Journal of Chemical Physics</i> , 2000, 113, 4250-4264. | 1.2 | 44 |
| 839 | Complete basis set extrapolations for low-lying triplet electronic states of acetylene and vinylidene. <i>Journal of Chemical Physics</i> , 2000, 113, 1447-1454. | 1.2 | 24 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 840 | A new complete basis set model (CBS-QB3) study on the possible intermediates in chemiluminescence. <i>Journal of Chemical Physics</i> , 2000, 113, 7731-7734. | 1.2 | 12 |
| 841 | Linear scaling computation of the Fock matrix. V. Hierarchical Cubature for numerical integration of the exchange-correlation matrix. <i>Journal of Chemical Physics</i> , 2000, 113, 10037-10043. | 1.2 | 43 |
| 842 | Autoionization-detected infrared spectroscopy of intramolecular hydrogen bonds in aromatic cations. II. Unconventional intramolecular hydrogen bonds. <i>Journal of Chemical Physics</i> , 2000, 112, 137-148. | 1.2 | 31 |
| 843 | Theoretical study of XONO ₂ (X=Br, OBr, O ₂ Br): Implications for stratospheric bromine chemistry. <i>Journal of Chemical Physics</i> , 2000, 113, 145-152. | 1.2 | 15 |
| 844 | Experimental and theoretical anharmonicity for benzene using density functional theory. <i>Journal of Chemical Physics</i> , 2000, 112, 248-259. | 1.2 | 135 |
| 845 | Crossed beam reaction of phenyl radicals with unsaturated hydrocarbon molecules. I. Chemical dynamics of phenylmethylacetylene (C ₆ H ₅ CCCH ₃ ;X \hat{a} \hat{e} \hat{s} 1A \hat{a} \hat{e} $\hat{2}$) formation from reaction of C ₆ H ₅ (X \hat{a} \hat{e} \hat{s} 2A ₁) with methylacetylene, CH ₃ CCH(X \hat{a} \hat{e} \hat{s} 1A ₁). <i>Journal of Chemical Physics</i> , 2000, 112, 4994-5001. | 1.2 | 32 |
| 846 | An assessment of theoretical methods for the study of transition metal carbonyl complexes: [Cl ₂ Rh(CO) ₂] \hat{a} \hat{r} and [Cl ₂ Rh(CO)] \hat{a} \hat{r} as case studies. <i>Journal of Chemical Physics</i> , 2000, 113, 9393-9401. | 1.2 | 23 |
| 847 | Photochemistry of Butatriene \hat{a} \hat{r} Spectroscopic Evidence for the Existence of Allenylcarbene \hat{e} . <i>Journal of Physical Chemistry A</i> , 2000, 104, 3819-3825. | 1.1 | 26 |
| 848 | Ligand close packing and the geometries of A(XY) ₄ and some related molecules. <i>Journal of Molecular Structure</i> , 2000, 520, 237-248. | 1.8 | 11 |
| 849 | Reactivity of CF _n (n=1 \hat{a} \hat{e} $\hat{3}$) species with a silica surface. <i>Surface Science</i> , 2000, 452, 117-124. | 0.8 | 0 |
| 850 | Adsorption of CO on MgO supported alkali monolayers: a periodic density functional local density approximation and generalized gradient approximation study. <i>Surface Science</i> , 2000, 445, 495-505. | 0.8 | 18 |
| 851 | Formation of Two Isomeric C ₃ HO Radicals from Charged Precursors in the Gas Phase. Potential Interstellar Molecules. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5817-5824. | 1.1 | 33 |
| 852 | Analytical calculation of nuclear magnetic resonance indirect spin \hat{e} spin coupling constants at the generalized gradient approximation and hybrid levels of density-functional theory. <i>Journal of Chemical Physics</i> , 2000, 113, 9402-9409. | 1.2 | 345 |
| 853 | Modeling Cytochrome Oxidase: A Quantum Chemical Study of the O \hat{a} \hat{r} O Bond Cleavage Mechanism. <i>Journal of the American Chemical Society</i> , 2000, 122, 12848-12858. | 6.6 | 112 |
| 854 | Kohn \hat{e} Sham calculations using hybrid exchange-correlation functionals with asymptotically corrected potentials. <i>Journal of Chemical Physics</i> , 2000, 113, 5185. | 1.2 | 31 |
| 855 | Assessment of Gaussian-3 and Density Functional Theories for Enthalpies of Formation of Cl \hat{a} \hat{r} C ₁₆ Alkanes. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5850-5854. | 1.1 | 231 |
| 856 | Heats of Formation for Cyclic C ₄ F _n , n= 4 \hat{a} \hat{r} 8, and Their Cations. <i>Journal of Physical Chemistry A</i> , 2000, 104, 9026-9028. | 1.1 | 10 |
| 857 | Photochemistry of 1H-Benzotriazole in Aqueous Solution: A Photolabile Base. <i>Journal of the American Chemical Society</i> , 2000, 122, 5849-5855. | 6.6 | 50 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|------|-----------|
| 858 | Experimental and Theoretical Investigation of the Mechanism of Radiation-Induced Radical Formation in Hydrogen-Bonded Cocrystals of 1-Methylcytosine and 5-Fluorouracil. <i>Journal of Physical Chemistry B</i> , 2000, 104, 9343-9350. | 1.2 | 26 |
| 859 | Electronic Structure of the 3d Metal Monoxide Anions. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5374-5379. | 1.1 | 102 |
| 860 | Theoretical Models for the Oxygen Radical Mechanism of Water Oxidation and of the Water Oxidizing Complex of Photosystem II. <i>Inorganic Chemistry</i> , 2000, 39, 2923-2935. | 1.9 | 154 |
| 861 | Computational Studies of the Mechanism for Proton and Hydride Transfer in Liver Alcohol Dehydrogenase. <i>Journal of the American Chemical Society</i> , 2000, 122, 4803-4812. | 6.6 | 168 |
| 862 | Hydroxyl Radical Reactions with Phenol as a Model for Generation of Biologically Reactive Tyrosyl Radicals. <i>Journal of Physical Chemistry B</i> , 2000, 104, 848-855. | 1.2 | 69 |
| 863 | Transition-Metal Systems in Biochemistry Studied by High-Accuracy Quantum Chemical Methods. <i>Chemical Reviews</i> , 2000, 100, 421-438. | 23.0 | 559 |
| 864 | QM ^{ab} /FE and Molecular Dynamics Calculations on Catechol O-Methyltransferase: Free Energy of Activation in the Enzyme and in Aqueous Solution and Regioselectivity of the Enzyme-Catalyzed Reaction. <i>Journal of the American Chemical Society</i> , 2000, 122, 2586-2596. | 6.6 | 87 |
| 865 | Conformational Studies in the Cyclohexane Series. 2. Phenylcyclohexane and 1-Methyl-1-phenylcyclohexane. <i>Journal of Organic Chemistry</i> , 2000, 65, 1181-1187. | 1.7 | 79 |
| 866 | Density Functional Theory Based Configuration Interaction Calculations on the Electronic Spectra of Free-Base Porphyrin, Chlorin, Bacteriochlorin, and cis- and trans-Isobacteriochlorin. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2504-2507. | 1.1 | 60 |
| 867 | Observation of a Stable Carbocation in a Consecutive Criegee Rearrangement with Trifluoroacetic Acid. <i>Journal of Organic Chemistry</i> , 2000, 65, 3926-3933. | 1.7 | 26 |
| 868 | Interfacial Electronic Structure in Thiolate Self-Assembled Monolayers: Implication for Molecular Electronics. <i>Journal of the American Chemical Society</i> , 2000, 122, 4700-4707. | 6.6 | 69 |
| 869 | Role of vibronic interactions in the electronic properties of a silicon cluster, (SiH) ₈ . <i>Journal of Chemical Physics</i> , 2000, 113, 2188-2198. | 1.2 | 13 |
| 870 | Synthesis, Characterization, and Theoretical Study of Stable Hydride [−] Azavinylidene Osmium(IV) Complexes. <i>Organometallics</i> , 2000, 19, 3100-3108. | 1.1 | 31 |
| 871 | Gas-Phase Coordination of Mg ⁺ , (c-C ₅ H ₅)Mg ⁺ , and (c-C ₅ H ₅) ₂ Mg ⁺ with Saturated Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2000, 104, 3926-3932. | 1.1 | 20 |
| 872 | Structure and Bonding of Transition Metal [−] Boryl Compounds. Theoretical Study of [(PH ₃) ₂ (CO)ClOs [−] BR ₂] and [(PH ₃) ₂ (CO) ₂ ClOs [−] BR ₂] (BR ₂ = BH ₂ , BF ₂ , B(OH) ₂ , B(OCHCHO), Bcat) [−] . <i>Inorganic Chemistry</i> , 2000, 39, 4776-4785. | 1.9 | 39 |
| 873 | Theoretical Studies of Some Transition-Metal-Mediated Reactions of Industrial and Synthetic Importance. <i>Chemical Reviews</i> , 2000, 100, 439-494. | 23.0 | 371 |
| 874 | Mixed Uranium Chloride Fluorides UF _{6-n} Cl _n and Methoxyuranium Fluorides UF _{6-n} (OCH ₃) _n : A Theoretical Study of Equilibrium Geometries, Vibrational Frequencies, and the Role of the f Orbitals. <i>Inorganic Chemistry</i> , 2000, 39, 1265-1274. | 1.9 | 28 |
| 875 | Stereoselective Reaction of [−] Sulfinyl Carbanion Derived from Chiral 2-(Trialkylsilyl)ethyl Sulfoxides: Evidence for a Novel Silicon [−] Oxygen Interaction. <i>Journal of Organic Chemistry</i> , 2000, 65, 469-474. | 1.7 | 19 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 876 | Metal vs Ligand Reduction in Complexes of 1,3-Dimethylalloxazine (DMA) with Copper(I), Ruthenium(II), and Tungsten(VI). Crystal Structures of (DMA)WO ₂ Cl ₂ and (Bis(1-methylimidazol-2-yl)ketone)WO ₂ Cl ₂ . <i>Inorganic Chemistry</i> , 2000, 39, 4052-4058. | 1.9 | 40 |
| 877 | Quadrupole coupling constants and isomeric Mössbauer shifts for inorganic compounds and complexes containing elements from period V calculated by ab initio methods. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 1877-1882. | 1.3 | 16 |
| 878 | The loss of CO from the ortho, meta and para forms of deprotonated methyl benzoate in the gas phase. <i>Perkin Transactions II RSC</i> , 2000, , 1665-1673. | 1.1 | 14 |
| 879 | Conversion of Linear to Rhombic C ₄ in the Gas Phase: A Joint Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2000, 122, 7105-7113. | 6.6 | 56 |
| 880 | Reaction-Path Dynamics Calculations of the NH ₃ + O(3P) Hydrogen Abstraction Reaction. <i>Journal of Physical Chemistry A</i> , 2000, 104, 7537-7544. | 1.1 | 25 |
| 881 | A Combined Spectroscopic and Theoretical Study of a Series of Aminomethyl End-Capped Oligothiophenes with Potential Applications in Thin Film Devices. <i>Journal of Physical Chemistry A</i> , 2000, 104, 735-740. | 1.1 | 24 |
| 882 | NMR Shielding Calculations across the Periodic Table: Diamagnetic Uranium Compounds. 1. Methods and Issues. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8244-8255. | 1.1 | 66 |
| 883 | Bond Dissociation Energies of the Tungsten Fluorides and Their Singly Charged Ions: A Density Functional Survey. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4077-4083. | 1.1 | 23 |
| 884 | A Study of the Products of the Reaction of Phosphorus and Dioxygen. <i>Journal of Physical Chemistry A</i> , 2000, 104, 3566-3571. | 1.1 | 22 |
| 885 | Oxidative Degradation of Pyruvate Formate-Lyase. <i>Journal of the American Chemical Society</i> , 2000, 122, 2035-2040. | 6.6 | 27 |
| 886 | Structure, Vibrational Absorption and Circular Dichroism Spectra, and Absolute Configuration of Tröger's Base. <i>Journal of the American Chemical Society</i> , 2000, 122, 2346-2354. | 6.6 | 79 |
| 887 | Electronic Structure of BCl Determined by Ab Initio Calculations and Resonance-Enhanced Multiphoton Ionization Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2000, 104, 3800-3805. | 1.1 | 17 |
| 888 | Ab Initio and Density Functional Study of the Activation Barrier for Ethane Cracking in Cluster Models of Zeolite H-ZSM-5. <i>Journal of Physical Chemistry B</i> , 2000, 104, 1944-1949. | 1.2 | 106 |
| 889 | Ab Initio Calculations on the 5-exo versus 6-endo Cyclization of 1,3-Hexadiene-5-yn-1-yl Radical: Formation of the First Aromatic Ring in Hydrocarbon Combustion. <i>Journal of the American Chemical Society</i> , 2000, 122, 11416-11422. | 6.6 | 20 |
| 890 | Conformations of Chiral Molecules in Solution: Ab Initio Vibrational Absorption and Circular Dichroism Studies of 4,4a,5,6,7,8-Hexahydro-4a-methyl-2(3H)-naphthalenone and 3,4,8,8a-Tetrahydro-8a-methyl-1,6(2H,7H)-naphthalenedione. <i>Journal of the American Chemical Society</i> , 2000, 122, 7358-7367. | 6.6 | 24 |
| 891 | Catalysis Mediated by Hydrogen Bonding: A Computational Study of the Aminolysis of 6-Chloropyrimidine. <i>Journal of the American Chemical Society</i> , 2000, 122, 5384-5386. | 6.6 | 8 |
| 892 | A Theoretical Study of the Radiationless Decay Mechanism of Cyclic Alkenes in the Lowest Triplet State. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5366-5373. | 1.1 | 11 |
| 893 | Reaction Path Hamiltonian Analysis of Dynamical Solvent Effects for a Claisen Rearrangement and a Diels-Alder Reaction. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8058-8066. | 1.1 | 37 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 894 | Reactivity of Gaseous XeF ⁺ Ions with Acetonitrile. A Joint Mass Spectrometric and Theoretical Study of Isomeric C ₂ H ₃ NF ⁺ and C ₂ H ₃ NXe ⁺ Cations. <i>Journal of Physical Chemistry A</i> , 2000, 104, 7574-7579. | 1.1 | 9 |
| 895 | Infrared Spectroscopy of Matrix-Isolated Polycyclic Aromatic Hydrocarbon Ions. 5. PAHs Incorporating a Cyclopentadienyl Ring. <i>Journal of Physical Chemistry A</i> , 2000, 104, 3655-3669. | 1.1 | 73 |
| 896 | Density Functional Studies of 19-Electron Organometallic Complexes: Investigation of Possible Ligand Distortions and Calculation of the EPR Parameters and Unpaired Electron Distributions in CpCr(CO) ₂ NO ⁻ , CpW(NO) ₂ P(OMe) ₃ , CpMo(CO) ₃ P(OMe) ₃ , and Co(CO) ₃ (2,3-bis(diphenylphosphino)maleic) Tj ETQq0 0 0 rgBT /Overlo | 1.1 | 14 |
| 897 | Theoretical Study of the Microsolvation of the Bromide Anion in Water, Methanol, and Acetonitrile: A Solvent vs Solvent-Solvent Interactions. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2799-2807. | 1.1 | 72 |
| 898 | Theoretical Studies of the Radiation Products of Hydroxyproline. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8583-8592. | 1.1 | 20 |
| 899 | Combined Theoretical and Vibrational Study of Dihexylbithienoquinonoid Derivatives with Regioregular Head-to-Head, Head-to-Tail, and Tail-to-Tail Orientations. <i>Journal of Physical Chemistry A</i> , 2000, 104, 661-672. | 1.1 | 30 |
| 900 | Is It Possible to Synthesize a Low-Valent Transition Metal Complex with a Neutral Carbon Atom as Terminal Ligand? A Theoretical Study of (CO) ₄ FeC. <i>Organometallics</i> , 2000, 19, 2698-2706. | 1.1 | 38 |
| 901 | Ligand Macrocyclic Structural Effects on Copper-Dioxygen Reactivity. <i>Inorganic Chemistry</i> , 2000, 39, 4059-4072. | 1.9 | 116 |
| 902 | Gas Phase Chemistry of NH _x Cl _y Ions. II. Structure, Stability and Reactivity of Protonated Dichloramine. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5617-5624. | 1.1 | 10 |
| 903 | TaFn and TaCl _n Atomization Energies for n = 1-5. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5843-5849. | 1.1 | 5 |
| 904 | Structure and Dynamics of [Nb(̂-5-C ₅ H ₄ SiMe ₃) ₂ (̂-2-H ₂ BR ₂)] (R ₂ = O ₂ C ₆ H ₄ , C ₈ H ₁₄ , H ₂) Complexes. A Combined Experimental and Theoretical Study. <i>Organometallics</i> , 2000, 19, 3654-3663. | 1.1 | 26 |
| 905 | Adiabatic Connection for Kinetics. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4811-4815. | 1.1 | 1,440 |
| 906 | A Density Functional Theory Study of the Radiation Products of Glycine. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5080-5086. | 1.1 | 36 |
| 907 | Matrix Infrared Spectra and Density Functional Calculations of Manganese and Rhenium Carbonyl Neutral and Anion Complexes. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8887-8897. | 1.1 | 32 |
| 908 | Vibrational Assignment of All 46 Fundamentals of C ₆₀ and C ₆₀ ⁻ : Scaled Quantum Mechanical Results Performed in Redundant Internal Coordinates and Compared to Experiments. <i>Journal of Physical Chemistry A</i> , 2000, 104, 102-112. | 1.1 | 86 |
| 909 | (N,N-Dimethylaminoxy)trifluorosilane: A Strong, Dipole Moment Driven Changes in the Molecular Geometry Studied by Experiment and Theory in Solid, Gas, and Solution Phases. <i>Journal of the American Chemical Society</i> , 2000, 122, 4471-4482. | 6.6 | 83 |
| 910 | Gas-Phase Vanadium Oxide Anions: Structure and Detachment Energies from Density Functional Calculations. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10913-10922. | 1.1 | 110 |
| 911 | Theoretical Studies of the Kinetic and Thermodynamic Stabilities of Isomers of HXGeS (X = H, F, Cl, and) Tj ETQq1 1,0,784314 rgBT /Ove | 1.1 | 11 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 912 | Bond Additivity Corrections for Quantum Chemistry Methods. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2168-2177. | 1.1 | 37 |
| 913 | A Computational Study of the Hydroxy-Group Directivity in the Peroxyformic Acid Epoxidation of the Chiral Allylic Alcohol (Z)-3-Methyl-3-penten-2-ol: A Control of Threo Diastereoselectivity through Allylic Strain and Hydrogen Bonding. <i>Journal of Organic Chemistry</i> , 2000, 65, 6715-6728. | 1.7 | 25 |
| 914 | Transition Regions in the Cope Rearrangement of 1,5-Hexadiene and Its Cyano Derivatives. <i>Journal of the American Chemical Society</i> , 2000, 122, 7377-7385. | 6.6 | 80 |
| 915 | Formation of Neutral C ₇ H ₂ Isomers from Four Isomeric C ₇ H ₂ Radical Anion Precursors in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2000, 104, 77-85. | 1.1 | 27 |
| 916 | Transient Hydrogen Atom Adducts to Disulfides. Formation and Energetics. <i>Journal of the American Chemical Society</i> , 2000, 122, 2361-2370. | 6.6 | 77 |
| 917 | A Mechanistic Study of Isopenicillin N Formation Using Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2000, 122, 8539-8547. | 6.6 | 31 |
| 918 | Heats of Formation for C _n F _m , C _n F _m ⁺ , CH _n F _m , and CH _n F _m ⁺ . <i>Journal of Physical Chemistry A</i> , 2000, 104, 4581-4585. | 1.1 | 29 |
| 919 | Can the Binuclear Dinitrogen Complex [P ₂ N ₂]Zr(1/4-1/2-N ₂)Zr[P ₂ N ₂] Activate More Than One Hydrogen Molecule? A Theoretical Study. <i>Organometallics</i> , 2000, 19, 3393-3403. | 1.1 | 32 |
| 920 | Structures, Vibrational Frequencies, and Normal Modes of Substituted Azo Dyes: Infrared, Raman, and Density Functional Calculations. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2734-2745. | 1.1 | 146 |
| 921 | A DFT/MRCI study on the excited state charge transfer states of N-pyrrolobenzene, N-pyrrolobenzonitrile and 4-N,N-dimethylaminobenzonitrile. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 5545-5552. | 1.3 | 77 |
| 922 | The Si ₂ Ci ₂ O (O ₂ Ci ₂ S) edward-lemieux effect is controlled by a P-orbital on oxygen. Evidence from electron momentum spectroscopy, photoelectron spectroscopy, X-ray crystallography, and density functional theory. <i>Israel Journal of Chemistry</i> , 2000, 40, 343-355. | 1.0 | 13 |
| 923 | Hartree-Fock and Density Functional Theory ab Initio Calculation of Optical Rotation Using GIAOs: Basis Set Dependence. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1039-1046. | 1.1 | 264 |
| 924 | Systematic Study of Oxo, Peroxo, and Superoxo Isomers of 3d-Metal Dioxides and Their Anions. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11961-11971. | 1.1 | 151 |
| 925 | Nature of the Chemical Bond between a Transition Metal and a Group-13 Element: Structure and Bonding of Transition Metal Complexes with Terminal Group-13 Diyl Ligands ER (E = B to Tl; R = Cp,) <i>J. Phys. Chem. A</i> 107:1314-1316 (2003) | 1.1 | 134 |
| 926 | Medium Polarization and Hydrogen Bonding Effects on Compound I of Cytochrome P450: What Kind of a Radical Is It Really?. <i>Journal of the American Chemical Society</i> , 2000, 122, 12892-12893. | 6.6 | 171 |
| 927 | Facile Synthesis of Alkynyl and Vinylidene Niobocene Complexes. Unexpected 1-Vinylidene-2-Alkyne Isomerization. <i>Organometallics</i> , 2000, 19, 1749-1765. | 1.1 | 32 |
| 928 | Assessment of Gaussian-3 and density functional theories for a larger experimental test set. <i>Journal of Chemical Physics</i> , 2000, 112, 7374-7383. | 1.2 | 711 |
| 929 | Rearrangements of 2-Nitrobenzyl Compounds. 1. Potential Energy Surface of 2-Nitrotoluene and Its Isomers Explored with ab Initio and Density Functional Theory Methods. <i>Journal of Physical Chemistry A</i> , 2000, 104, 7856-7870. | 1.1 | 75 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|------|-----------|
| 930 | Hydrogen Atom Adducts to Nitrobenzene: Formation of the Phenylnitronic Radical in the Gas Phase and Energetics of Wheland Intermediates. <i>Journal of the American Chemical Society</i> , 2000, 122, 9511-9524. | 6.6 | 62 |
| 931 | Can Hydrocarbon Chains Be Disrupted by Fast O(3P) Atoms?. <i>Journal of Physical Chemistry A</i> , 2000, 104, 9976-9982. | 1.1 | 28 |
| 932 | Computational electrochemistry: aqueous one-electron oxidation potentials for substituted anilines. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 1231-1239. | 1.3 | 194 |
| 933 | Activation of Small Alkanes in Ga-Exchanged Zeolites: A Quantum Chemical Study of Ethane Dehydrogenation. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2468-2475. | 1.1 | 82 |
| 934 | Reactivity of Alkyl versus Silyl Peroxides. The Consequences of 1,2-Silicon Bridging on the Epoxidation of Alkenes with Silyl Hydroperoxides and Bis(trialkylsilyl)peroxides. <i>Journal of Organic Chemistry</i> , 2000, 65, 8629-8639. | 1.7 | 21 |
| 935 | Enhanced Aromaticity of the Transition Structures for the Diels-Alder Reactions of Quinodimethanes: Evidence from ab Initio and DFT Computations. <i>Journal of Organic Chemistry</i> , 2000, 65, 7971-7976. | 1.7 | 56 |
| 936 | Mechanism of the Olefin Epoxidation Catalyzed by Molybdenum Diperoxo Complexes: Quantum-Chemical Calculations Give an Answer to a Long-Standing Question. <i>Journal of the American Chemical Society</i> , 2000, 122, 10101-10108. | 6.6 | 128 |
| 937 | Syntheses of NCN and NC3N from Ionic Precursors in the Gas Phase and an Unusual Rearrangement of Neutral NC3N: A Joint Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11248-11256. | 1.1 | 35 |
| 938 | Corannulene as a Lewis Base: Computational Modeling of Protonation and Lithium Cation Binding. <i>Journal of the American Chemical Society</i> , 2001, 123, 6687-6695. | 6.6 | 67 |
| 939 | Neural-network analysis of the vibrational spectra of N-acetyl-L-alanyl-L-methyl amide conformational states. <i>Physical Review E</i> , 2001, 64, 021905. | 0.8 | 18 |
| 940 | High Level Ab Initio Calculations of the Optical Gap of Small Silicon Quantum Dots. <i>Physical Review Letters</i> , 2001, 87, 276402. | 2.9 | 156 |
| 941 | Ab Initio Calculation of Amide Carbonyl Stretch Vibrational Frequencies in Solution with Modified Basis Sets. 1. N-Methyl Acetamide. <i>Journal of Physical Chemistry A</i> , 2001, 105, 10922-10928. | 1.1 | 184 |
| 942 | Modeling of radical-surface interactions in the plasma-enhanced chemical vapor deposition of silicon thin films. <i>Advances in Chemical Engineering</i> , 2001, 28, 251-296. | 0.5 | 36 |
| 943 | (V2O5) _n Gas-Phase Clusters (n = 1-12) Compared to V2O5 Crystal: DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8588-8598. | 1.1 | 135 |
| 944 | High Coverages of Hydrogen on a (10,0) Carbon Nanotube. <i>Nano Letters</i> , 2001, 1, 223-226. | 4.5 | 95 |
| 945 | The Intrinsic Stability of the Noble Gas-Coordinated Transition-Metal Complex Ions. <i>Journal of the American Chemical Society</i> , 2001, 123, 2340-2343. | 6.6 | 38 |
| 946 | The enthalpy of formation of dibenzofuran and some related oxygen-containing heterocycles in the gas phase. A GAUSSIAN-3 theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 3717-3721. | 1.3 | 12 |
| 947 | Spectroscopic and Theoretical Investigations of Vibrational Frequencies in Binary Unsaturated Transition-Metal Carbonyl Cations, Neutrals, and Anions. <i>Chemical Reviews</i> , 2001, 101, 1931-1962. | 23.0 | 427 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 948 | DimesitylketoneO-Oxide: Spectroscopic Characterization, Conformation, and Reaction Modes: OH Formation and OH Capture. <i>Journal of the American Chemical Society</i> , 2001, 123, 2618-2627. | 6.6 | 25 |
| 949 | Kinetic and Density Functional Studies on Alkyl-Carbene Elimination from PdIIHeterocyclic Carbene Complexes: A New Type of Reductive Elimination with Clear Implications for Catalysis. <i>Journal of the American Chemical Society</i> , 2001, 123, 4029-4040. | 6.6 | 232 |
| 950 | Ab initioCompton maps of small molecules. <i>Molecular Physics</i> , 2001, 99, 175-186. | 0.8 | 7 |
| 951 | A Theoretical Study of the Dynamic Behavior of Alkane Hydroxylation by a Compound I Model of Cytochrome P450. <i>Journal of the American Chemical Society</i> , 2001, 123, 9806-9816. | 6.6 | 97 |
| 952 | Calculation of Optical Rotation Using Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5356-5371. | 1.1 | 351 |
| 953 | Molecular Dynamics Simulations and Spectroscopic Studies of Amorphous Tetraglyme (CH ₃ O(CH ₂ CH ₂ O) ₄ CH ₃) and Tetraglyme:LiCF ₃ SO ₃ Structures. <i>Journal of Physical Chemistry B</i> , 2001, 105, 3329-3337. | 1.2 | 41 |
| 954 | Theoretical Study of the Photophysics of Adenine in Solution: Tautomerism, Deactivation Mechanisms, and Comparison with the 2-Aminopurine Fluorescent Isomer. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4749-4757. | 1.1 | 123 |
| 955 | A Theoretical Study of the Chorismate Synthase Reaction. <i>Organic Letters</i> , 2001, 3, 4137-4140. | 2.4 | 13 |
| 956 | Differentiation of Î²-Sheet-Forming Structures: Ab Initio-Based Simulations of IR Absorption and Vibrational CD for Model Peptide and Protein Î²-Sheets. <i>Journal of the American Chemical Society</i> , 2001, 123, 12048-12058. | 6.6 | 295 |
| 957 | How Well Can Hybrid Density Functional Methods Predict Transition State Geometries and Barrier Heights?. <i>Journal of Physical Chemistry A</i> , 2001, 105, 2936-2941. | 1.1 | 558 |
| 958 | Mechanism of the Addition Reaction of Alkyl Azides to [60]Fullerene and the Subsequent N ₂ Extrusion to Form Monoimino-[60]fullerenes. <i>Journal of Organic Chemistry</i> , 2001, 66, 433-442. | 1.7 | 91 |
| 959 | Mechanisms for the incorporation of a nitrogen atom into polycyclic aromatic hydrocarbon cations. <i>Chemical Physics Letters</i> , 2001, 347, 473-480. | 1.2 | 23 |
| 960 | The Theoretical Prediction of Molecular Radical Species: a Systematic Study of Equilibrium Geometries and Harmonic Vibrational Frequencies. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9736-9747. | 1.1 | 142 |
| 961 | A Quantum Chemical Approach to the Study of Reaction Mechanisms of Redox-Active Metalloenzymes. <i>Journal of Physical Chemistry B</i> , 2001, 105, 9375-9386. | 1.2 | 101 |
| 962 | A combined ab initio and photoelectron study of galena (PbS). <i>Surface Science</i> , 2001, 491, 226-238. | 0.8 | 36 |
| 963 | Nitrobenzene Isomers. <i>Journal of Physical Chemistry A</i> , 2001, 105, 995-1010. | 1.1 | 20 |
| 964 | Hydride shift in substituted phenyl glyoxals: Interpretation of experimental rate data using electronic structure and variational transition state theory calculations. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 3967-3972. | 1.3 | 3 |
| 965 | Theory predicts that the weaker Î€-accepting ligand diaminoborylene occupies the equatorial position in (OC) ₄ FeÎ€B(NH ₂): theoretical study of (OC) ₄ FeÎ€B(NH ₂) and (OC) ₄ FeÎ€BHÎ€S. <i>Dalton Transactions RSC</i> . 2001, , 434-440. | | 62 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 966 | The unusual neutral OCOCO and possible charged analogues. A theoretical investigation. Perkin Transactions II RSC, 2001, , 2244-2247. | 1.1 | 11 |
| 967 | A time-resolved infrared spectroscopic study of $[M(\text{SnR}_3)_2(\text{CO})_2(\text{diimine})]$ ($M = \text{Ru, Os}$; $R = \text{Ph, Me}$): evidence of charge redistribution in the lowest-excited state. Dalton Transactions RSC, 2001, , 2587-2592. | 2.3 | 16 |
| 968 | Glyoxal studied with $\hat{\text{e}}^{\text{TM}}$, explicit large amplitude motion and anharmonicity. Physical Chemistry Chemical Physics, 2001, 3, 1958-1964. | 1.3 | 21 |
| 969 | A DFT study of Zr-S rotational barriers of $(\text{i-C}_5\text{H}_5)_2\text{Zr}(\text{Cl})(\text{SR})$; the origin of an inverse steric effect. Canadian Journal of Chemistry, 2001, 79, 809-816. | 0.6 | 2 |
| 970 | EVALUATION OF SEVERAL ECONOMICAL COMPUTATIONAL METHODS FOR GEOMETRY OPTIMISATION OF PHOSPHORUS ACID DERIVATIVES. Nucleosides, Nucleotides and Nucleic Acids, 2001, 20, 1381-1384. | 0.4 | 4 |
| 971 | Molecular dynamics simulations of plastoquinone in solution. Molecular Physics, 2001, 99, 247-253. | 0.8 | 16 |
| 972 | Unprecedented C-H bond oxidative addition of the imidazolium cation to Pt0: a combined density functional analysis and experimental study. Chemical Communications, 2001, , 355-356. | 2.2 | 122 |
| 973 | A novel anion rearrangement. The conversion of $[\text{CC}(\text{O})(\text{CN})]^-$ to $[\text{NCCCO}]^-$ in the gas phase: a joint experimental and theoretical study. Perkin Transactions II RSC, 2001, , 827-831. | 1.1 | 8 |
| 974 | Structure and Bonding in Dinuclear Oxoanions of V, Nb, Ta, Mo, and W. Journal of Physical Chemistry A, 2001, 105, 7111-7117. | 1.1 | 26 |
| 975 | Regioselectivity in 2-Methylbutane Hydroxylation Mediated by FeO^+ and FeO_2^+ . Organometallics, 2001, 20, 1397-1407. | 1.1 | 20 |
| 976 | A Theoretical Study of the Effect of a Tetraalkylammonium Counterion on the Hydrogen Bond Strength in Z-Hydrogen Maleate. Journal of the American Chemical Society, 2001, 123, 7134-7145. | 6.6 | 35 |
| 977 | Energetics of Uracil Cation Radical and Anion Radical Ion-Molecule Reactions in the Gas Phase. Journal of Physical Chemistry A, 2001, 105, 8740-8747. | 1.1 | 18 |
| 978 | On the regioselectivity of nucleophilic additions to anisole- $\text{Cr}(\text{CO})_3$ and related complexes: a density functional study. New Journal of Chemistry, 2001, 25, 446-450. | 1.4 | 16 |
| 979 | Solvent Effects on the Reaction Coordinate of the Hydrolysis of Phosphates and Sulfates: Application of Hammond and Anti-Hammond Postulates to Understand Hydrolysis in Solution. Journal of the American Chemical Society, 2001, 123, 11755-11763. | 6.6 | 53 |
| 980 | DFT study of the structural and redox properties of $[\text{Cp}_2\text{Fe}_2\text{S}_4]_q$ complexes ($q = 0, +2, +1$ and -2). New Journal of Chemistry, 2001, 25, 611-617. | 1.4 | 13 |
| 981 | The Substrate Reaction Mechanism of Class III Anaerobic Ribonucleotide Reductase. Journal of Physical Chemistry B, 2001, 105, 6445-6452. | 1.2 | 19 |
| 982 | Stability and Bonding Situation of Electron-Deficient Transition-Metal Complexes. Theoretical Study of the CO-Labilizing Effect of Ligands L in $[\text{W}(\text{CO})_5\text{L}]$ ($L = \text{C}_2\text{H}_2, \text{NCH}, \text{N}_2, \text{C}_2\text{H}_4, \text{OH}_2, \text{SH}_2, \text{NH}_3, \text{F}, \text{Cl},$) Tj ETQq0,0,0 rgBT /Overlock 1 Complexes $[\text{W}(\text{CO})_4\text{L}]$ and $[\text{W}(\text{CO})_3\text{L}]_2$. Organometallics, 2001, 20, 2510-2524. | 1.1 | 34 |
| 983 | Arene-Mercury Complexes Stabilized Aluminum and Gallium Chloride: Synthesis and Structural Characterization. Journal of the American Chemical Society, 2001, 123, 11219-11228. | 6.6 | 34 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 984 | Systematic Study of the Quality of Various Quantum Similarity Descriptors. Use of the Autocorrelation Function and Principal Component Analysis. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8805-8814. | 1.1 | 32 |
| 985 | Multi-coefficient Correlation Method: A Comparison of Specific-Range Reaction Parameters to General Parameters for C _n H _x O _y Compounds. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4143-4149. | 1.1 | 15 |
| 986 | Dynamics of Photosubstitution Reactions of Fe(CO) ₅ : An Ultrafast Infrared Study of High Spin Reactivity. <i>Journal of the American Chemical Society</i> , 2001, 123, 6909-6915. | 6.6 | 66 |
| 987 | Theoretical Study of Guanine from Gas Phase to Aqueous Solution: Role of Tautomerism and Its Implications in Absorption and Emission Spectra. <i>Journal of Physical Chemistry A</i> , 2001, 105, 7126-7134. | 1.1 | 82 |
| 988 | Formaldehyde Oxime \rightleftharpoons Nitrosomethane Tautomerism. <i>Journal of Organic Chemistry</i> , 2001, 66, 6762-6767. | 1.7 | 70 |
| 989 | Ab Initio Study of the Two Iso-electronic Molecules NpO ₄ ⁻ and UO ₄ ²⁻ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 10570-10576. | 1.1 | 28 |
| 990 | Structural and Electronic Properties of an Azamacrocyclic, C ₂₆ H ₁₈ N ₆ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 8500-8503. | 1.1 | 4 |
| 991 | The Triplet Potential Energy Surface of s-trans-2,4-Hexadiene. A Comparison of Theory and Experiment. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3934-3939. | 1.1 | 13 |
| 992 | Density Functional Theory Calculation of Molecular Structure and Vibrational Spectra of Dibenzothiophene in the Ground and the Lowest Triplet State. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8093-8097. | 1.1 | 13 |
| 993 | A Density Functional Study of the Reactivity and Stability of Mixed Copper Complexes. Is Hardness the Reason?. <i>Inorganic Chemistry</i> , 2001, 40, 301-306. | 1.9 | 10 |
| 994 | CS ₂ Fixation by Carbonic Anhydrase Model Systems: A New Substrate in the Catalytic Cycle. <i>Inorganic Chemistry</i> , 2001, 40, 1006-1013. | 1.9 | 23 |
| 995 | Direct Observation of a Hydrogen Atom Adduct to C-5 in Uracil. A Neutralization-Reionization Mass Spectrometric and ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8339-8351. | 1.1 | 26 |
| 996 | Unexpected Nitrosyl-Group Bending in Six-Coordinate {M(NO)} ₆ -Bonded Aryl(iron) and -(ruthenium) Porphyrins. <i>Journal of the American Chemical Society</i> , 2001, 123, 6314-6326. | 6.6 | 104 |
| 997 | Computational Analysis of the Autocatalytic Posttranslational Cyclization Observed in Histidine Ammonia-Lyase. A Comparison with Green Fluorescent Protein. <i>Journal of the American Chemical Society</i> , 2001, 123, 4679-4686. | 6.6 | 25 |
| 998 | A Density Functional Study on the Effect of the Trans Axial Ligand of Cobalamin on the Homolytic Cleavage of the Co-C Bond. <i>Journal of Physical Chemistry B</i> , 2001, 105, 7564-7571. | 1.2 | 74 |
| 999 | Direct Observation of a Hydrogen Atom Adduct to O-4 in Uracil. Energetics and Kinetics of Uracil Radicals. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8352-8360. | 1.1 | 35 |
| 1000 | Unraveling the Origin of Regioselectivity in Rhodium Diphosphine Catalyzed Hydroformylation. A DFT QM/MM Study. <i>Journal of the American Chemical Society</i> , 2001, 123, 7630-7637. | 6.6 | 141 |
| 1001 | Gas-Phase Reactivity of Ni ⁺ with Glycine. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5340-5347. | 1.1 | 66 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1002 | Dinuclear Trivalent and Mixed-Valence Uranium [(η^5 -CH ₂) ₅]4-calix[4]tetrapyrrole Complexes with Short Intermetallic Distances. <i>Organometallics</i> , 2001, 20, 5440-5445. | 1.1 | 38 |
| 1003 | An Experimental and Computational Study on the Reactivity and Regioselectivity for the Nitrosoarene Ene Reaction: A Comparison with Triazolinedione and Singlet Oxygen. <i>Journal of the American Chemical Society</i> , 2001, 123, 5542-5548. | 6.6 | 45 |
| 1004 | Quantum Mechanical Dynamics of Hydride Transfer in Polycyclic Hydroxy Ketones in the Condensed Phase. <i>Journal of the American Chemical Society</i> , 2001, 123, 1459-1463. | 6.6 | 11 |
| 1005 | A Consecutive Double-Criegee Rearrangement Using TFPA: A Stepwise Conversion of Homoadamantane to Oxahomoadamantanes. <i>Journal of Organic Chemistry</i> , 2001, 66, 1701-1707. | 1.7 | 15 |
| 1006 | EPR Characteristics of the [(NC) ₅ M(NO)] ³⁺ -Ions (M = Fe, Ru, Os). Experimental and DFT Study Establishing NO as a Ligand. <i>Inorganic Chemistry</i> , 2001, 40, 5704-5707. | 1.9 | 87 |
| 1007 | g- and A-Tensor Calculations in the Zero-Order Approximation for Relativistic Effects of Ni Complexes and Ni(CO) ₃ H as Model Complexes for the Active Center of [NiFe]-Hydrogenase. <i>Journal of Physical Chemistry A</i> , 2001, 105, 416-425. | 1.1 | 64 |
| 1008 | On the Origin of Nonvertical Triplet Excitation Transfer: The Relative Role of Double-Bond and Phenyl-Vinyl Torsions in the Stilbenes. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6273-6276. | 1.1 | 27 |
| 1009 | Reactions of a Hexahydride ²⁺ Osmium Complex with Aromatic Ketones: C-H Activation versus C-F Activation. <i>Organometallics</i> , 2001, 20, 442-452. | 1.1 | 88 |
| 1010 | (Salen)Mn(III)-Catalyzed Epoxidation Reaction as a Multichannel Process with Different Spin States. Electronic Tuning of Asymmetric Catalysis: A Theoretical Study. <i>Inorganic Chemistry</i> , 2001, 40, 4040-4048. | 1.9 | 82 |
| 1011 | Modeling the Action of an Antitumor Drug: A Density Functional Theory Study of the Mechanism of Tirapazamine. <i>Journal of the American Chemical Society</i> , 2001, 123, 7320-7325. | 6.6 | 23 |
| 1012 | Hydrogen-Bond Mediated Catalysis: The Aminolysis of 6-Chloropyrimidine as Catalyzed by Derivatives of Uracil. <i>Journal of the American Chemical Society</i> , 2001, 123, 2047-2052. | 6.6 | 8 |
| 1013 | Synthesis and Characterization of Mixed-Phosphine Osmium Polyhydrides: Hydrogen Delocalization in [OsH ₅ P ₃] ⁺ Systems. <i>Organometallics</i> , 2001, 20, 5297-5309. | 1.1 | 20 |
| 1014 | Molecular Structure of Substituted Phenylamine $\hat{\pm}$ -OMe- and $\hat{\pm}$ -OH-p-Benzoquinone Derivatives. Synthesis and Correlation of Spectroscopic, Electrochemical, and Theoretical Parameters. <i>Journal of Organic Chemistry</i> , 2001, 66, 8349-8363. | 1.7 | 58 |
| 1015 | Bonding of Rare-Gas Atoms to Si in Reactions of Rare Gases with SiF ₃ ⁺ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 11073-11079. | 1.1 | 25 |
| 1016 | Triplet Organometallic Reactivity under Ambient Conditions: An Ultrafast UV Pump/IR Probe Study. <i>Journal of the American Chemical Society</i> , 2001, 123, 2255-2264. | 6.6 | 82 |
| 1017 | A quantum chemistry approach for current-voltage characterization of molecular junctions. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 5017-5023. | 1.3 | 95 |
| 1018 | Cyclizations of Enynes Catalyzed by PtCl ₂ or Other Transition Metal Chlorides: Divergent Reaction Pathways. <i>Journal of the American Chemical Society</i> , 2001, 123, 10511-10520. | 6.6 | 305 |
| 1019 | A New Sulfur Oxide, OSOSO, and Its Cation, Likely Present in the Io's Atmosphere: Detection and Characterization by Mass Spectrometric and Theoretical Methods. <i>Journal of the American Chemical Society</i> , 2001, 123, 478-484. | 6.6 | 24 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1020 | Ionization of Atmospheric Gases Containing Ozone and Carbonyl Sulfide. Formation and Reactivity of SO ⁺ Ions. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1144-1149. | 1.1 | 8 |
| 1021 | Hydrogen Atom Adducts to the Amide Bond. Generation and Energetics of the Amino(hydroxy)methyl Radical in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2001, 105, 11144-11155. | 1.1 | 47 |
| 1022 | Formation of CH ₃ CFCl ⁺ from Photoionization of CH ₃ CFCl ₂ : An Application of Threshold Photoelectron Photoion Coincidence (TPEPICO) Technique. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1226-1231. | 1.1 | 7 |
| 1023 | Hydroxyl Radical Adducts to Pyridine. The Generation and Properties of the Elusive N-Hydroxypyridyl Radical. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9130-9141. | 1.1 | 14 |
| 1024 | Protonation of an H ₂ O Dimer by a Zeolitic Brønsted Acid Site. <i>Journal of Physical Chemistry B</i> , 2001, 105, 3034-3038. | 1.2 | 29 |
| 1025 | Ruthenium ^{II} Aminoallylidene Complexes from Butatrienyliene Intermediates via an Aza-Cope Rearrangement: Synthetic, Spectroscopic, Electrochemical, Spectroelectrochemical, and Computational Studies. <i>Organometallics</i> , 2001, 20, 1317-1333. | 1.1 | 73 |
| 1026 | Infrared Spectroscopy of the OH Stretching Vibrations of Jet-Cooled Salicylic Acid and Its Dimer in S ₀ and S ₁ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 10673-10680. | 1.1 | 59 |
| 1027 | Donor and Acceptor Properties of the Chromium Tricarbonyl Substituent in Benzylic and Homobenzylic Anions, Cations, and Radicals. <i>Journal of Organic Chemistry</i> , 2001, 66, 6738-6744. | 1.7 | 33 |
| 1028 | Infrared Photodissociation Spectroscopy of n-Propylbenzene ⁺ Ar Cluster Cations: Charge Delocalization between the Aromatic Ring and the Alkyl Chain. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4882-4886. | 1.1 | 9 |
| 1029 | Mechanism of Ring-Opening Polymerization of 1,5-Dioxepan-2-one and L-Lactide with Stannous 2-Ethylhexanoate. A Theoretical Study. <i>Macromolecules</i> , 2001, 34, 3877-3881. | 2.2 | 164 |
| 1030 | Femtosecond Infrared Study of the Dynamics of Solvation and Solvent Caging. <i>Journal of the American Chemical Society</i> , 2001, 123, 4204-4210. | 6.6 | 36 |
| 1031 | Molecular dynamics simulations of ubiquinone; a survey over torsional potentials and hydrogen bonds. <i>Molecular Physics</i> , 2001, 99, 1795-1804. | 0.8 | 15 |
| 1032 | Intramolecular Rearrangements in Six-Coordinate Ruthenium and Iron Dihydrides. <i>Inorganic Chemistry</i> , 2001, 40, 620-627. | 1.9 | 25 |
| 1033 | The vibrations of glyoxal, studied by ϵ -Multimode TM , with a large amplitude motion, using an ab initio potential surface. <i>Molecular Physics</i> , 2001, 99, 393-402. | 0.8 | 16 |
| 1034 | Selectivity in Gas-Phase Ion Chemistry. Competitive Fast Reactions in a Silane/Propene System. <i>Organometallics</i> , 2001, 20, 4593-4599. | 1.1 | 10 |
| 1035 | Mechanisms for enzymatic reactions involving formation or cleavage of O-O bonds. <i>Theoretical and Computational Chemistry</i> , 2001, , 95-143. | 0.2 | 2 |
| 1036 | Catalytic Reactions of Radical Enzymes. <i>Theoretical and Computational Chemistry</i> , 2001, 9, 145-181. | 0.2 | 0 |
| 1037 | Insertion Aptitudes and Insertion Regiochemistry of Various Alkenes Coordinated to Cationic (<i>i</i> -R)(diimine)palladium(II) (R = \sim CH ₃ , \sim C ₆ H ₅). A Theoretical Study. <i>Organometallics</i> , 2001, 20, 2813-2819. | 1.1 | 81 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1038 | Reparameterization of hybrid functionals based on energy differences of states of different multiplicity. <i>Theoretical Chemistry Accounts</i> , 2001, 107, 48-55. | 0.5 | 1,240 |
| 1039 | Stabilization of diazene in Fe(II)-sulfur model complexes relevant for nitrogenase activity. I. A new approach to the evaluation of intramolecular hydrogen bond energies. <i>Theoretical Chemistry Accounts</i> , 2001, 106, 379-392. | 0.5 | 57 |
| 1040 | Density-functional investigation of bonding in tetrahedral MO ₄ anions. <i>Polyhedron</i> , 2001, 20, 2269-2277. | 1.0 | 51 |
| 1041 | A density functional approach of prototropic tautomerism of guanine. <i>Chemical Physics</i> , 2001, 264, 187-196. | 0.9 | 26 |
| 1042 | Empty levels probed by XAS and ETS in cyclic polymethylene sulfides (CH ₂) _n S, n=2,3,4,5. <i>Chemical Physics</i> , 2001, 265, 105-112. | 0.9 | 10 |
| 1043 | Ab initio and density functional theory calculation of the structure and vibrational properties of n-vertex closo-carboranes, n=5, 6 and 7. <i>Chemical Physics</i> , 2001, 271, 17-30. | 0.9 | 18 |
| 1044 | Vibronic interaction in a copper oxide cluster. <i>Chemical Physics</i> , 2001, 271, 31-39. | 0.9 | 0 |
| 1045 | Structure and reactivity of the vinylcyclopropane radical cation. <i>Journal of Molecular Structure</i> , 2001, 599, 95-116. | 1.8 | 6 |
| 1046 | Spectroscopy and photochemical reactivity of cyclooctadiene platinum complexes. <i>Journal of Organometallic Chemistry</i> , 2001, 620, 202-210. | 0.8 | 27 |
| 1047 | Synthesis and characterization of 2,5,7-trichalcogena-1,3,4,6-tetrasilanorbornanes (RMeSiSiMe) ₂ E ₃ (R=Me, Ph/E=S, Se, Te). <i>Journal of Organometallic Chemistry</i> , 2001, 627, 144-152. | 0.8 | 27 |
| 1048 | Group 14 chalcogenides featuring a bicyclo[3.3.0]octane skeleton. <i>Journal of Organometallic Chemistry</i> , 2001, 630, 139-148. | 0.8 | 32 |
| 1049 | Olefin strain energies and platinum complexes of highly pyramidalised alkenes. <i>Journal of Organometallic Chemistry</i> , 2001, 635, 142-152. | 0.8 | 10 |
| 1050 | Applications of neural network prediction of conformational states for small peptides from spectra and of fold classes. <i>Computers & Chemistry</i> , 2001, 26, 65-77. | 1.2 | 4 |
| 1051 | Determination of absolute configuration using vibrational circular dichroism spectroscopy: the chiral sulfoxide 1-thiochroman S-oxide. <i>Tetrahedron: Asymmetry</i> , 2001, 12, 1551-1558. | 1.8 | 42 |
| 1052 | An ab initio study of adsorption related properties of diatomic molecules in zeolites. <i>Journal of Molecular Catalysis A</i> , 2001, 166, 175-187. | 4.8 | 20 |
| 1053 | Fragment mode analysis and its application to the vibrational normal modes of boron trichloride-ammonia and boron trichloride-pyridine complexes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2001, 57, 521-534. | 2.0 | 5 |
| 1054 | Closed-shell polycyclic aromatic hydrocarbon cations: a new category of interstellar polycyclic aromatic hydrocarbons. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2001, 57, 907-930. | 2.0 | 107 |
| 1055 | Electron energy loss and dissociative electron attachment spectroscopy of methyl vinyl ether and related compounds. <i>International Journal of Mass Spectrometry</i> , 2001, 205, 43-55. | 0.7 | 15 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1056 | Sigma bond activation by transition metal ions: the Co(CH ₄) _n ⁺ systems revisited. <i>International Journal of Mass Spectrometry</i> , 2001, 204, 281-294. | 0.7 | 24 |
| 1057 | Fe(CH ₄) _n ⁺ and Ni(CH ₄) _n ⁺ clusters: experimental and theoretical bond energies for n = 1-6. <i>International Journal of Mass Spectrometry</i> , 2001, 210-211, 265-281. | 0.7 | 36 |
| 1058 | Pyrimidine-ylidenes produced using neutralization-reionization mass spectrometry and probed by density functional methods. <i>International Journal of Mass Spectrometry</i> , 2001, 210-211, 43-57. | 0.7 | 20 |
| 1059 | Loss of CO ₂ from the ortho isomer of deprotonated methyl phenyl carbonate involves a methyl migration. <i>International Journal of Mass Spectrometry</i> , 2001, 210-211, 557-562. | 0.7 | 2 |
| 1060 | Cyclization of acylium ions with nitriles: gas-phase synthesis and characterization of 1,3,5-oxadiazinium ions. <i>International Journal of Mass Spectrometry</i> , 2001, 212, 445-454. | 0.7 | 22 |
| 1061 | Unexpectedly large basis set effects on the binding of O ₂ to heme complexes. <i>International Journal of Quantum Chemistry</i> , 2001, 85, 100-108. | 1.0 | 10 |
| 1062 | Ab initio modeling of competitive drug-drug interactions: 5-fluorouracil dimers in the gas phase and in solution. <i>International Journal of Quantum Chemistry</i> , 2001, 83, 128-142. | 1.0 | 11 |
| 1063 | B3LYP studies of the formation of neutral tyrosyl radical Yz [•] and regeneration of neutral tyrosine Yz in PSII. <i>International Journal of Quantum Chemistry</i> , 2001, 83, 220-229. | 1.0 | 15 |
| 1064 | Henry constants predicted using multipole expansion for the interaction energies. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 58-69. | 1.0 | 7 |
| 1065 | Gas-phase electrophilic fluorination of methanol by XeF ⁺ . Formation and characterization of protonated methyl hypofluorite and hypoxenite. <i>Journal of Mass Spectrometry</i> , 2001, 36, 392-396. | 0.7 | 8 |
| 1066 | Computational chemistry: A useful (sometimes mandatory) tool in mass spectrometry studies. <i>Mass Spectrometry Reviews</i> , 2001, 20, 195-245. | 2.8 | 160 |
| 1067 | A new mechanism for initiation of free-radical chain reactions during high-temperature, homogeneous oxidation of unsaturated hydrocarbons: Ethylene, propyne, and allene. <i>International Journal of Chemical Kinetics</i> , 2001, 33, 698-706. | 1.0 | 28 |
| 1068 | Theoretical study of the mechanism of peptide ring formation in green fluorescent protein. <i>International Journal of Quantum Chemistry</i> , 2001, 81, 169-186. | 1.0 | 30 |
| 1069 | Ab initio calculations on XF _n q (X = I, Xe, Cs, and Ba; n=1, 2, 4, and 6; q=?1, 0, +1, and +2) molecules. <i>International Journal of Quantum Chemistry</i> , 2001, 81, 238-245. | 1.0 | 2 |
| 1070 | Distorted silicon hydrides? a comparative study with various density functionals. <i>Journal of Computational Chemistry</i> , 2001, 22, 151-161. | 1.5 | 12 |
| 1071 | The para-didehydropyridine, para-didehydropyridinium, and related biradicals? a contribution to the chemistry of enediyne antitumor drugs. <i>Journal of Computational Chemistry</i> , 2001, 22, 216-229. | 1.5 | 64 |
| 1072 | A Computational Study of the Mechanisms for the Incorporation of a Nitrogen Atom into Polycyclic Aromatic Hydrocarbons in the Titan Haze. <i>Icarus</i> , 2001, 154, 516-521. | 1.1 | 79 |
| 1073 | When anomeric effects collide. <i>Journal of Computational Chemistry</i> , 2001, 22, 1194-1204. | 1.5 | 20 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1074 | Gas-phase detection of the HBCC (X1?) molecule: a combined crossed beam and computational study of the B(2P)+C2H2(1?g+) reaction. <i>Journal of Computational Chemistry</i> , 2001, 22, 1359-1365. | 1.5 | 24 |
| 1075 | CationicClosoCarboranes-Promising Weakly Coordinating Ions. <i>Journal of Computational Chemistry</i> , 2001, 22, 1542-1551. | 1.5 | 13 |
| 1076 | On the interaction of Mo and Mo2 with NH3, C2H4, and C3H6. <i>Journal of Computational Chemistry</i> , 2001, 22, 1557-1564. | 1.5 | 11 |
| 1077 | Modeling aspects of mechanisms for reactions catalyzed by metalloenzymes. <i>Journal of Computational Chemistry</i> , 2001, 22, 1634-1645. | 1.5 | 127 |
| 1078 | Parametrization of the Becke3-LYP hybrid functional for a series of small molecules using quantum molecular similarity techniques. <i>Journal of Computational Chemistry</i> , 2001, 22, 1666-1678. | 1.5 | 21 |
| 1079 | syn~anti Conversion in Octahedral Bis(Î²-diketonato)diorganotin(IV) Derivatives Containing Fluorinated 4-Acyl-5-pyrazolonato Donors. <i>European Journal of Inorganic Chemistry</i> , 2001, 2001, 2171-2180. | 1.0 | 15 |
| 1082 | An Experimental and Theoretical Study of the Basicity of Tetra-tert-butyltetrahedrane. <i>Chemistry - A European Journal</i> , 2001, 7, 342-346. | 1.7 | 27 |
| 1083 | The Reaction Rate Constant of Chlorine Nitrate Hydrolysis. <i>Chemistry - A European Journal</i> , 2001, 7, 1662-1669. | 1.7 | 11 |
| 1084 | Dinuclear Diazene Iron and Ruthenium Complexes as Models for Studying Nitrogenase Activity. <i>Chemistry - A European Journal</i> , 2001, 7, 5195-5202. | 1.7 | 54 |
| 1085 | Dicyclopenta[a,d]cyclooctene: A [14]Annulene Containing Two Zero-Atom Cross-Links. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 2660-2662. | 7.2 | 14 |
| 1086 | PtII-Catalyzed Intramolecular Reaction of Furans with Alkynes. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 4754-4757. | 7.2 | 132 |
| 1087 | O-H Bond Dissociation Energies of Phenolic Compounds are Determined by Field/Inductive Effect or Resonance Effect?A DFT Study and Its Implication. <i>QSAR and Combinatorial Science</i> , 2001, 20, 148-152. | 1.4 | 49 |
| 1088 | On the integration accuracy in molecular density functional theory calculations using Gaussian basis sets. <i>Computer Physics Communications</i> , 2001, 133, 189-201. | 3.0 | 116 |
| 1089 | Resonance Raman spectra of d6 metal-â€œdiimine complexes reflect changes in metal-â€œligand interaction and character of electronic transition. <i>Coordination Chemistry Reviews</i> , 2001, 219-221, 937-955. | 9.5 | 27 |
| 1090 | Calculation of frequency dependent optical rotation using density functional response theory. <i>Chemical Physics Letters</i> , 2001, 339, 380-388. | 1.2 | 158 |
| 1091 | Assessment of a new local exchange functional OPTX. <i>Chemical Physics Letters</i> , 2001, 341, 319-328. | 1.2 | 472 |
| 1092 | Quantum mechanical tunneling in methylamine dehydrogenase. <i>Chemical Physics Letters</i> , 2001, 347, 512-518. | 1.2 | 57 |
| 1093 | On the reaction CH2NH2++HCN/HNCâ†’NH2CH2CNH+. <i>Chemical Physics Letters</i> , 2001, 346, 267-273. | 1.2 | 13 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1094 | Using hydrogen and chlorine on Si(111) to store data, an improved model. <i>Chemical Physics Letters</i> , 2001, 347, 291-296. | 1.2 | 4 |
| 1095 | Is the Lamb shift chemically significant?. <i>Chemical Physics Letters</i> , 2001, 348, 497-500. | 1.2 | 28 |
| 1096 | Heats of formation for Fe(CO) _n (n=1-4). <i>Chemical Physics Letters</i> , 2001, 350, 313-317. | 1.2 | 15 |
| 1097 | Hybrid quantum mechanics/molecular mechanics studies of the active site of the blue copper proteins amicyanin and rusticyanin. <i>Inorganica Chimica Acta</i> , 2001, 324, 21-26. | 1.2 | 30 |
| 1098 | Nitromethyl Radical, Cation, and Anion. A Neutralization and Electron Photodetachment Reionization Mass Spectrometric and ab Initio Computational Study of [C,H2,N,O2] Isomers. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1371-1382. | 1.1 | 15 |
| 1099 | Metabolism of Sirolimus and Its Derivative Everolimus by Cytochrome P450 3A4: Insights from Docking, Molecular Dynamics, and Quantum Chemical Calculations. <i>Journal of Medicinal Chemistry</i> , 2001, 44, 2027-2034. | 2.9 | 60 |
| 1100 | Oxidative Addition of the Imidazolium Cation to Zerovalent Ni, Pd, and Pt: A Combined Density Functional and Experimental Study. <i>Journal of the American Chemical Society</i> , 2001, 123, 8317-8328. | 6.6 | 242 |
| 1101 | Title is missing!. <i>International Journal of Thermophysics</i> , 2001, 22, 1813-1831. | 1.0 | 1 |
| 1102 | Theoretical determination of the vibrational absorption and Raman spectra of 3-methylindole and 3-methylindole radicals. <i>Chemical Physics</i> , 2001, 265, 13-25. | 0.9 | 29 |
| 1103 | Imaging of orbital electron densities by electron momentum spectroscopy – a chemical interpretation of the binary (e,2e) reaction. <i>Chemical Physics</i> , 2001, 270, 13-30. | 0.9 | 70 |
| 1104 | The reaction of polycyclic aromatic hydrocarbon anions with hydrogen. <i>Chemical Physics</i> , 2001, 274, 11-14. | 0.9 | 14 |
| 1105 | Previtamin D conformations and the wavelength-dependent photoconversions of previtamin D. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2001, 139, 125-131. | 2.0 | 15 |
| 1106 | Dynamic behavior of hydrogen bonding in hydrogen 5,6-acenaphthenedicarboxylate. <i>Tetrahedron</i> , 2001, 57, 7263-7268. | 1.0 | 2 |
| 1107 | Using hydrogen and chlorine on Si(111) to store data. <i>Chemical Physics Letters</i> , 2001, 333, 1-5. | 1.2 | 7 |
| 1108 | On the reaction CH ₂ O+NH ₃ →CH ₂ NH+H ₂ O. <i>Chemical Physics Letters</i> , 2001, 333, 6-11. | 1.2 | 17 |
| 1109 | A discrete variable representation study of the dynamics of the double proton transfer in bicyclic oxalamidines. <i>Chemical Physics Letters</i> , 2001, 340, 591-596. | 1.2 | 4 |
| 1110 | Ab initio MO investigation on the reactivity for electrophilic substitution of phenolics with oxirane and aziridine, as the model compounds of binding site of mutagen. <i>Computational and Theoretical Chemistry</i> , 2001, 536, 73-82. | 1.5 | 12 |
| 1111 | Thermochemical analysis of the OH+C ₂ H ₄ →C ₂ H ₄ OH reaction using accurate theoretical methods. <i>Computational and Theoretical Chemistry</i> , 2001, 537, 199-212. | 1.5 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 1112 | Calculation of static mean polarisability and polarisability anisotropy. Statistical comparison with the results of gases and influence of the geometrical parameters. Computational and Theoretical Chemistry, 2001, 542, 167-176. | 1.5 | 11 |
| 1113 | Density functional theory study of the conformation and energetics of silanol and disiloxane. Computational and Theoretical Chemistry, 2001, 542, 227-237. | 1.5 | 39 |
| 1114 | DFT study of L±-alanine as a function of the medium polarity. Computational and Theoretical Chemistry, 2001, 544, 151-157. | 1.5 | 12 |
| 1115 | A B3LYP study of intramolecular hydrogen bonding and proton transfer in naphthazarin: a model system for daunomycin/adriamycin. Computational and Theoretical Chemistry, 2001, 549, 123-136. | 1.5 | 25 |
| 1116 | Model calculations of radiation induced damage in 1-methylthymine:9-methyladenine. Computational and Theoretical Chemistry, 2001, 549, 55-61. | 1.5 | 3 |
| 1117 | TiO ₂ -photocatalyzed degradation of phenol and ortho-substituted phenolic compounds. Applied Catalysis B: Environmental, 2001, 30, 359-373. | 10.8 | 200 |
| 1118 | Disrotatory and Conrotatory Transition Structures for the Fe(CO) ₃ -Templated Rearrangement of Methylene cyclopropane to Trimethylenemethane. Organometallics, 2001, 20, 4562-4564. | 1.1 | 20 |
| 1119 | Density Functional Theory, Methods, Techniques, and Applications. , 2001, , 105-160. | | 1 |
| 1120 | Generation of Free Radicals by Emodic Acid and its [d-Lys6]GnRH-conjugate. Photochemistry and Photobiology, 2001, 74, 226. | 1.3 | 24 |
| 1121 | S ₃ O, a new sulfur oxide identified in the gas phase. Chemical Communications, 2001, , 2086-2087. | 2.2 | 14 |
| 1122 | The performance of density functional theory for equilibrium molecular properties of symmetry breaking molecules. Journal of Chemical Physics, 2001, 114, 8257-8269. | 1.2 | 39 |
| 1123 | Competition between agostic WCH ₂ ⁺ and HWCH ⁺ : A joint experimental and theoretical study. Journal of Chemical Physics, 2001, 115, 2510-2518. | 1.2 | 22 |
| 1124 | Electronic structure of halogen-substituted methyl radicals: Excited states of CH ₂ Cl and CH ₂ F. Journal of Chemical Physics, 2001, 115, 7485-7494. | 1.2 | 17 |
| 1125 | A multifacet mechanism for the OH+HNO ₃ reaction: An ab initio molecular orbital/statistical theory study. Journal of Chemical Physics, 2001, 114, 4522. | 1.2 | 28 |
| 1126 | Infrared and density-functional-theory study of spherosiloxane-based model silicon/silicon oxide interfaces. Physical Review B, 2001, 64, . | 1.1 | 11 |
| 1127 | Photodissociation dynamics of the CH ₂ Cl radical: Ion imaging studies of the Cl+CH ₂ channel. Journal of Chemical Physics, 2001, 115, 7474-7484. | 1.2 | 18 |
| 1128 | Density functional theory predictions of anharmonicity and spectroscopic constants for diatomic molecules. Journal of Chemical Physics, 2001, 115, 2439-2448. | 1.2 | 39 |
| 1129 | Emphasizing the exchange-correlation potential in functional development. Journal of Chemical Physics, 2001, 114, 3958-3967. | 1.2 | 40 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1130 | Efficiency of the π -conjugation in a novel family of C_{18} -bisphenyl end-capped oligothiophenes by means of Raman spectroscopy. <i>Journal of Chemical Physics</i> , 2002, 116, 10419-10427. | 1.2 | 63 |
| 1131 | Are the maximum hardness and minimum polarizability principles always obeyed in nontotally symmetric vibrations?. <i>Journal of Chemical Physics</i> , 2002, 117, 10561-10570. | 1.2 | 77 |
| 1132 | Velocity map imaging of ion-molecule reaction products: $\text{Co}^+(3F_4) + \text{isobutane}$. <i>Journal of Chemical Physics</i> , 2002, 117, 653-665. | 1.2 | 24 |
| 1133 | Phosphorous trapped within buckminsterfullerene. <i>Journal of Chemical Physics</i> , 2002, 116, 7849-7854. | 1.2 | 54 |
| 1134 | Coupled-cluster Raman intensities: Assessment and comparison with multiconfiguration and density functional methods. <i>Journal of Chemical Physics</i> , 2002, 117, 8623-8633. | 1.2 | 39 |
| 1135 | First-principles studies of the structural and electronic properties of pyrite FeS_2 . <i>Physical Review B</i> , 2002, 65, . | 1.1 | 64 |
| 1136 | 2A $\tilde{\Sigma}^-$ and 2A $\tilde{\Sigma}^+$ Energy Surfaces for the $\text{Sc} + \text{CO}_2 \rightarrow \text{ScO} + \text{CO}$ Reaction. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9551-9557. | 1.1 | 39 |
| 1137 | The Relation Between Polyhedral Borane Sandwiches and Endohedral Complexes; the Electronic Structure and Stability of $\text{X}@\text{YmBnHn+m}^q$ ($\text{X} = \text{He, Ne, Li, Be}$; $\text{Y} = \text{B, C, Si}$; $m = 0-3$; $n = 12-9$; $q = -2$ to $+2$), $(\text{C}_2\text{B}_4\text{H}_6)_2\text{X}^q$ ($\text{X} = \text{Li, Al, Si}$; $q = -3, -1, 0$) and $\text{X}_2@\text{B}_{17}\text{H}_{17}^q$ ($\text{X} = \text{He, Li}$; $q = -2, 0$). <i>Collection of Czechoslovak Chemical Communications</i> , 2002, 67, 965-990. | 1.0 | 10 |
| 1138 | Reductive Damage in Directly Ionized DNA: Saturation of the C_5C_6 Bond of Cytosine in d(CGCG) $_2$ Crystals. <i>Radiation Research</i> , 2002, 157, 235-242. | 0.7 | 18 |
| 1139 | Theoretical Study of Dimethyl Maleate and Its Complexes with Lewis Acids: Effect of the Interaction between Two Methoxycarbonyl Groups on Equilibrium Structures. <i>Bulletin of the Chemical Society of Japan</i> , 2002, 75, 1785-1793. | 2.0 | 5 |
| 1140 | Comparison of Some Computational Methods for Geometry Optimisation of Phosphorus Acid Derivatives. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2002, 177, 2711-2724. | 0.8 | 4 |
| 1141 | Protonated Carbonic Acid and the Trihydroxymethyl Radical in the Gas Phase. A Neutralization-Recombination Mass Spectrometric and ab Initio/RRKM Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5938-5950. | 1.1 | 20 |
| 1142 | Theoretical Study of Methyl-PdII-N-Heterocyclic Silylene and Germylene Complexes: Comparisons to N-Heterocyclic Carbene Reactivity. <i>Organometallics</i> , 2002, 21, 5408-5414. | 1.1 | 27 |
| 1143 | Mechanism for the Formaldehyde to Formic Acid and the Formic Acid to Carbon Dioxide Conversions Mediated by an Iron-Oxo Species. <i>Journal of Physical Chemistry A</i> , 2002, 106, 621-630. | 1.1 | 31 |
| 1144 | Theoretical Study on Chlorine and Hydrogen Shift in Cycloheptatriene and Cyclopentadiene Derivatives. <i>Journal of Organic Chemistry</i> , 2002, 67, 625-632. | 1.7 | 42 |
| 1145 | Structures and Relative Energies of Polylithiated Benzenes. <i>Journal of Organic Chemistry</i> , 2002, 67, 7389-7398. | 1.7 | 19 |
| 1146 | Reaction-Path Dynamics Calculations Using Integrated Methods. The $\text{CF}_3\text{CH}_3 + \text{OH}$ Hydrogen Abstraction Reaction. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5686-5696. | 1.1 | 18 |
| 1147 | Arene-Mercury Complexes Stabilized by Gallium Chloride: Relative Rates of H/D and Arene Exchange. <i>Journal of the American Chemical Society</i> , 2002, 124, 14156-14161. | 6.6 | 22 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1148 | First-Principles Determination of the Absolute Hydration Free Energy of the Hydroxide Ion. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9737-9744. | 1.1 | 105 |
| 1149 | Dynamics of 1,2-Hydrogen Migration in Carbenes and Ring Expansion in Cyclopropylcarbenes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5323-5338. | 1.1 | 46 |
| 1150 | A Density Functional Theory Approach to the Development of QM Parameters for the Prediction of Reactivity in Free-Radical Copolymerizations. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10311-10325. | 1.1 | 29 |
| 1151 | Direct C-C Bond Breaking in the Reaction of O(3P) with Fluoropolymers in Low Earth Orbit. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5463-5467. | 1.1 | 28 |
| 1152 | Molecular Structures and Excited States of CpM(CO) ₂ (Cp = η^5 -C ₅ H ₅ ; M = Rh, Ir) and [Cl ₂ Rh(CO) ₂] ⁻ . Theoretical Evidence for a Competitive Charge Transfer Mechanism. <i>Journal of the American Chemical Society</i> , 2002, 124, 2664-2671. | 6.6 | 27 |
| 1153 | New Empirical Procedures for Improving ab Initio Energetics. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9910-9917. | 1.1 | 8 |
| 1154 | Reactions of HOCl + HCl + nH ₂ O and HOCl + HBr + nH ₂ O. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7850-7857. | 1.1 | 19 |
| 1155 | Lactone Enols Are Stable in the Gas Phase but Highly Unstable in Solution. <i>Journal of the American Chemical Society</i> , 2002, 124, 13282-13289. | 6.6 | 11 |
| 1156 | Isolation and Characterization of Four Isomers of a C ₆₀ Bisadduct with a TTF Derivative. Study of Their Radical Ions. <i>Journal of Organic Chemistry</i> , 2002, 67, 566-575. | 1.7 | 22 |
| 1157 | Theoretical Studies of the Cross-Linking Mechanisms between Cytosine and Tyrosine. <i>Journal of the American Chemical Society</i> , 2002, 124, 2753-2761. | 6.6 | 35 |
| 1158 | Electronic Structure of Halogen-Substituted Methyl Radicals: Equilibrium Geometries and Vibrational Spectra of CH ₂ Cl and CH ₂ F. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5169-5176. | 1.1 | 14 |
| 1159 | Multitask Molecular Springs: Collective Helical Vibrations of R ₂ Sn (R = H, C ₆ H ₅ , C ₂ H ₃ , CCl ₃) A Quantum Mechanical Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1661-1669. | 1.1 | 3 |
| 1160 | Solvation of Sulfur-Centered Cations and Anions in Acetonitrile. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8827-8833. | 1.1 | 23 |
| 1161 | An ab Initio Study of the Interaction of SCN ⁻ with a Silver Electrode: The Prediction of Vibrational Frequencies. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1450-1457. | 1.1 | 37 |
| 1162 | A Mechanism from Quantum Chemical Studies for Methane Formation in Methanogenesis. <i>Journal of the American Chemical Society</i> , 2002, 124, 4039-4049. | 6.6 | 125 |
| 1163 | Electronic and Steric Ligand Effects on the Activity and Regiochemistry in the Heck Reaction. <i>Organometallics</i> , 2002, 21, 2248-2253. | 1.1 | 43 |
| 1164 | Vanadium Insertion into CO ₂ , CS ₂ and OCS: A Comparative Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4181-4186. | 1.1 | 49 |
| 1165 | Origin of Bonding Interactions in Cu ₂ +(H ₂) _n Clusters: An Experimental and Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10027-10032. | 1.1 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1166 | Raman Spectra and Normal Coordinate Analysis of the N1 [~] H and N3 [~] H Tautomers of 4-Methylimidazole: δ Vibrational Modes of Histidine Tautomer Markers. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3403-3412. | 1.1 | 42 |
| 1167 | Vibrational Circular Dichroism within the Polarizable Continuum Model: A Theoretical Evidence of Conformation Effects and Hydrogen Bonding for (S)-(1 [~])-3-Butyn-2-ol in CCl ₄ Solution. <i>Journal of Physical Chemistry A</i> , 2002, 106, 12331-12339. | 1.1 | 83 |
| 1168 | Inverse Isotope Effects of a Late Transition Metal Olefin Polymerization Catalyst: A DFT Study. <i>Organometallics</i> , 2002, 21, 4950-4954. | 1.1 | 15 |
| 1169 | Helicoid Shiftamers. <i>Journal of the American Chemical Society</i> , 2002, 124, 6836-6837. | 6.6 | 11 |
| 1170 | Theoretical Study of the Reaction XY ₄ = XY ₃ + Y, Where X = C, Si, Ge, Sn, Pb and Y = CH ₃ , C ₂ H ₅ . <i>Journal of Physical Chemistry A</i> , 2002, 106, 7057-7061. | 1.1 | 6 |
| 1171 | Spectroelectrochemical Raman Study of Two End-Capped Sexithiophenes with Applications as Electroactive Molecular Materials. <i>Journal of Physical Chemistry B</i> , 2002, 106, 2488-2496. | 1.2 | 37 |
| 1172 | Participation of Co-Ligands in Electronic Transitions of Platinum(II) Diazabutadiene Complexes. <i>Inorganic Chemistry</i> , 2002, 41, 5216-5225. | 1.9 | 20 |
| 1173 | Density Functional Theory Study of Alkali Metal [~] Noble Metal Diatomic Molecules. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11637-11643. | 1.1 | 30 |
| 1174 | Computational Probes into the Basis of Silver Ion Chromatography. II. Silver(I) [~] Olefin Complexes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11197-11204. | 1.1 | 44 |
| 1175 | Theoretical and Experimental Study of the Vibrational Spectra of the $\hat{1}\pm$, $\hat{1}^2$, and $\hat{1}^r$ Phases of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). <i>Journal of Physical Chemistry B</i> , 2002, 106, 10594-10604. | 1.2 | 71 |
| 1176 | Electronic Structure of the $\hat{1}\pm$ and $\hat{1}^2$ Isomers Of [Mo ₈ O ₂₆] ⁴⁻ . <i>Inorganic Chemistry</i> , 2002, 41, 3500-3507. | 1.9 | 51 |
| 1177 | Why Does Cp ₂ YH Catalyze the Polymerization of Ethene but Not of Propene?. <i>Organometallics</i> , 2002, 21, 1861-1869. | 1.1 | 6 |
| 1178 | An Infrared Study of δ -Hydrogen Bonds in Micro-solvated Phenol: OH Stretching Vibrations of Phenol [~] X (X = C ₆ H ₆ , C ₂ H ₄ , and C ₂ H ₂) Clusters in the Neutral and Cationic Ground States. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8554-8560. | 1.1 | 76 |
| 1179 | Vibrational Spectra of Vinylarsine and Vinylstibine. An Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6262-6270. | 1.1 | 6 |
| 1180 | Vibrational Spectroscopic Features of a Novel Family of Amorphous Molecular Materials Containing an Oligothiophene Moiety as Color-Tunable Emitting Materials. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7163-7170. | 1.2 | 41 |
| 1181 | The Spin Distribution in Low-Spin Iron Porphyrins. <i>Journal of the American Chemical Society</i> , 2002, 124, 11771-11780. | 6.6 | 64 |
| 1182 | Kinetics and Mechanism of the OH + C ₆ H ₆ Reaction: A Detailed Analysis with First-Principles Calculations. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11309-11326. | 1.1 | 89 |
| 1183 | Three-Dimensional Structure Determination of N-(p-Tolyl)-dodecylsulfonamide from Powder Diffraction Data and Validation of Structure Using Solid-State NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2002, 124, 14450-14459. | 6.6 | 33 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1184 | Structures and Enthalpies of Formation in the Gas Phase of the Most Toxic Polychlorinated Dibenzop-dioxins. A DFT Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6618-6627. | 1.1 | 23 |
| 1185 | Reductive Dechlorination of 1,1,2,2-Tetrachloroethane. <i>Environmental Science & Technology</i> , 2002, 36, 3536-3541. | 4.6 | 79 |
| 1186 | Thionyl Fluoride from Sulfur Hexafluoride Corona Discharge Decomposition: Gas-Phase Chemistry of [SOF ₂] ⁺ H ⁺ Ions. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9261-9266. | 1.1 | 12 |
| 1187 | Computational Studies on the Isomeric Structures in the Pyrophosphito Bridged Diplatinum(II) Complex, Platinum Pop. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7617-7620. | 1.1 | 13 |
| 1188 | Gas-Phase Basicity of 2,7-Dimethyl-[1,2,4]-Triazepine Thio Derivatives. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7383-7389. | 1.1 | 18 |
| 1189 | Atom Scrambling of Linear C ₅ in the Gas Phase: a Joint Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1374-1380. | 1.1 | 15 |
| 1190 | Two- and Four-Electron Alkyne Ligands in Osmium ⁺ Cyclopentadienyl Chemistry: Consequences of the π - σ Interaction. <i>Organometallics</i> , 2002, 21, 305-314. | 1.1 | 54 |
| 1191 | Global Hardness Evaluation Using Simplified Models for the Hardness Kernel. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4632-4638. | 1.1 | 29 |
| 1192 | Substituent Effects in the Interconversion of Phenylcarbene, Bicyclo[4.1.0]hepta-2,4,6-triene, and 1,2,4,6-Cycloheptatetraene. <i>Journal of Organic Chemistry</i> , 2002, 67, 2532-2540. | 1.7 | 32 |
| 1193 | N-Amination of Peptides: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1441-1449. | 1.1 | 14 |
| 1194 | Gauge-Origin Independent Density-Functional Theory Calculations of Vibrational Raman Optical Activity. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7448-7455. | 1.1 | 162 |
| 1195 | The Formation of the Neutral Isomers NCCCCO and CCC(O)CN in the Gas Phase from Ionic Precursors: a Joint Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10470-10476. | 1.1 | 5 |
| 1196 | Theoretical Study of the Interaction of Water and Imidazole with Iron and Nickel Dications. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3219-3223. | 1.1 | 18 |
| 1197 | A Density-Functional Study of the Mechanism for the Diastereoselective Epoxidation of Chiral Allylic Alcohols by the Titanium Peroxy Complexes. <i>Journal of Organic Chemistry</i> , 2002, 67, 1427-1435. | 1.7 | 27 |
| 1198 | Toward the Spectrum of Free Polyethylene: Linear Alkanes Studied by Carbon 1s Photoelectron Spectroscopy and Theory. <i>Journal of the American Chemical Society</i> , 2002, 124, 7866-7873. | 6.6 | 41 |
| 1199 | Quantum Chemical Study of Degenerate Hydride Shifts in Acyclic Tertiary Carbocations. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1604-1611. | 1.1 | 43 |
| 1200 | Relationship between Molecular Structure and Electron Targets in the Electroreduction of Benzocarbazolidiones and Anilinaphthoquinones. Experimental and Theoretical Study. <i>Journal of Organic Chemistry</i> , 2002, 67, 3673-3681. | 1.7 | 37 |
| 1201 | Neutral versus Charged Species in Enzyme Catalysis. Classical and Free Energy Barriers for Oxygen Atom Transfer from C ₄ a-Hydroperoxyflavin to Dimethyl Sulfide. <i>Journal of Organic Chemistry</i> , 2002, 67, 8653-8661. | 1.7 | 26 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1202 | Diverse Evolution of $[\{\text{Ph}_2\text{P}(\text{CH}_2)_n\text{PPh}_2\}\text{Pt}(\text{S})_2\text{Pt}\{\text{Ph}_2\text{P}(\text{CH}_2)_n\text{PPh}_2\}]$ ($n = 2, 3$) Metalloligands in CH_2Cl_2 . <i>Inorganic Chemistry</i> , 2002, 41, 3218-3229. | 1.9 | 50 |
| 1203 | Keto-Enol Isomerization of Acetaldehyde in HZSM5. A Theoretical Study Using the ONIOM2 Method. <i>Journal of Physical Chemistry B</i> , 2002, 106, 10220-10226. | 1.2 | 46 |
| 1204 | QUANTUMMECHANICALMETHODS FORENZYMEKINETICS. <i>Annual Review of Physical Chemistry</i> , 2002, 53, 467-505. | 4.8 | 730 |
| 1205 | Theoretical Study of the $\text{Fe}(\text{phen})_2(\text{NCS})_2$ Spin-Crossover Complex with Reparametrized Density Functionals. <i>Inorganic Chemistry</i> , 2002, 41, 6928-6935. | 1.9 | 411 |
| 1206 | Determination of the Structures of Chiral Molecules Using Vibrational Circular Dichroism Spectroscopy. <i>ACS Symposium Series</i> , 2002, , 18-33. | 0.5 | 22 |
| 1207 | Density Functional Study of the Proline-Catalyzed Direct Aldol Reaction. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5155-5159. | 1.1 | 188 |
| 1208 | Structure and Bonding in $[\text{W}_{10}\text{O}_{32}]_n$ -Isopolyanions. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6114-6120. | 1.1 | 23 |
| 1209 | A Birch-like Mechanism in Enzymatic Benzoyl-CoA Reduction: A Kinetic Study of Substrate Analogues Combined with an ab Initio Model. <i>Biochemistry</i> , 2002, 41, 1752-1758. | 1.2 | 57 |
| 1210 | Effect of Geminal Substitution on the Strain Energy of Dioxiranes. Origin of the Low Ring Strain of Dimethyldioxirane. <i>Journal of Organic Chemistry</i> , 2002, 67, 3884-3896. | 1.7 | 58 |
| 1211 | A Computational Study of the Isomerization of Prolyl Amides As Catalyzed by Intramolecular Hydrogen Bonding. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11168-11172. | 1.1 | 23 |
| 1212 | A hybrid density functional theory study of the low-temperature dimethyl ether combustion pathways. I: Chain-propagation. <i>Israel Journal of Chemistry</i> , 2002, 42, 245-260. | 1.0 | 25 |
| 1213 | Polarizabilities of Solvents from the Chemical Composition. <i>Journal of Chemical Information and Computer Sciences</i> , 2002, 42, 1154-1163. | 2.8 | 171 |
| 1214 | Configurational and Conformational Analysis of Chiral Molecules Using IR and VCD Spectroscopies: Spiropentylcarboxylic Acid Methyl Ester and Spiropentyl Acetate. <i>Journal of Organic Chemistry</i> , 2002, 67, 8090-8096. | 1.7 | 52 |
| 1215 | A DFT and HF quantum chemical study of the tin nanocluster $[(\text{R}_3\text{Sn})_{12}\text{O}_{14}(\text{OH})_6]^{2+}$ and its interactions with anions and neutral nucleophiles: confrontation with experimental data. <i>New Journal of Chemistry</i> , 2002, 26, 1108-1117. | 1.4 | 18 |
| 1216 | Assertion and validation of the performance of the B3LYP functional for the first transition metal row and the G2 test set. <i>Journal of Chemical Physics</i> , 2002, 117, 4729-4737. | 1.2 | 534 |
| 1217 | A Comparative Theoretical Study on DMABN: Significance of Excited State Optimized Geometries and Direct Comparison of Methodologies. <i>Journal of Physical Chemistry A</i> , 2002, 106, 804-815. | 1.1 | 65 |
| 1218 | Nitro derivatives of pyrrole, furan and 1H-tetrazole: ring or nitro bases?. <i>New Journal of Chemistry</i> , 2002, 26, 1567-1574. | 1.4 | 14 |
| 1219 | Heats of formation of phosphorus compounds determined by current methods of computational quantum chemistry. <i>Journal of Chemical Physics</i> , 2002, 117, 11175-11187. | 1.2 | 40 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 1220 | Arene π -Mercury Complexes Stabilized by Aluminum and Gallium Chloride: π Catalysts for H/D Exchange of Aromatic Compounds. <i>Journal of the American Chemical Society</i> , 2002, 124, 3743-3748. | 6.6 | 20 |
| 1221 | Charge Model 3: π A Class IV Charge Model Based on Hybrid Density Functional Theory with Variable Exchange. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10707-10717. | 1.1 | 48 |
| 1222 | A density functional theory study of phosphorescence and triplet π -triplet absorption for nonlinear absorption chromophores. <i>Journal of Chemical Physics</i> , 2002, 117, 7128-7136. | 1.2 | 67 |
| 1223 | Electrophilic Addition of Ph ₃ PAu ⁺ to Anionic Alkoxy Fischer-Type Carbene Complexes: π A Novel Approach to Metal-Stabilized Bimetallic Vinyl Ether Complexes. <i>Organometallics</i> , 2002, 21, 3173-3181. | 1.1 | 46 |
| 1224 | The electronic states of Fe ₂ S ₂ π /0/+2+. <i>Journal of Chemical Physics</i> , 2002, 116, 617-628. | 1.2 | 44 |
| 1225 | Structure and thermochemistry of Fe ₂ S ₂ π /0/+gas phase clusters and their fragments. B3LYP calculations. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5234-5243. | 1.3 | 47 |
| 1226 | Spin π -spin coupling tensors by density-functional linear response theory. <i>Journal of Chemical Physics</i> , 2002, 117, 5998-6009. | 1.2 | 70 |
| 1227 | Lithium π -Benzene Sandwich Compounds: π A Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9533-9537. | 1.1 | 41 |
| 1228 | Direct Observation of Weak Hydrogen Bonds in Microsolvated Phenol: Infrared Spectroscopy of OH Stretching Vibrations of Phenol π -CO and π -CO ₂ in S ₀ and D ₀ . <i>Journal of Physical Chemistry A</i> , 2002, 106, 10124-10129. | 1.1 | 47 |
| 1229 | Infrared Spectra and Density Functional Theory Calculations on Transition Metal Nitrosyls. Vibrational Frequencies of Unsaturated Transition Metal Nitrosyls. <i>Chemical Reviews</i> , 2002, 102, 885-912. | 23.0 | 296 |
| 1230 | Searching for the Second Oxidant in the Catalytic Cycle of Cytochrome P450: π A Theoretical Investigation of the Iron(III)-Hydroperoxo Species and Its Epoxidation Pathways. <i>Journal of the American Chemical Society</i> , 2002, 124, 2806-2817. | 6.6 | 295 |
| 1231 | Structures, Metal π -Ligand Bond Strength, and Bonding Analysis of Ferrocene Derivatives with Group-15 Heteroligands Fe(π -5-E) ₂ and FeCp(π -5-E) (E = N, P, As, Sb). A Theoretical Study π . <i>Organometallics</i> , 2002, 21, 3351-3359. | 1.1 | 129 |
| 1232 | Cycloaddition Reactions of Acrylonitrile on the Si(100)-2 \times 1 Surface. <i>Journal of the American Chemical Society</i> , 2002, 124, 6162-6167. | 6.6 | 43 |
| 1233 | The calculation of structural, elastic and phase stability properties of minerals using first principles techniques: A comparison of HF, DFT and Hybrid functional treatments of exchange and correlation. <i>Molecular Simulation</i> , 2002, 28, 903-915. | 0.9 | 15 |
| 1234 | Analysis of the effect of changing the α 0 parameter of the Becke3-LYP hybrid functional on the transition state geometries and energy barriers in a series of prototypical reactions. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 722-731. | 1.3 | 51 |
| 1235 | Chlorophylla Radical Ions: π A Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2002, 106, 5281-5288. | 1.2 | 23 |
| 1236 | Nonstatistical Translational Energy Distribution of H ₂ Elimination Products from Co ⁺ (3F ₄) + Propane. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5563-5576. | 1.1 | 32 |
| 1237 | Reaction Space Map Representation of the Chlorination/Dechlorination Reactions of Polychlorobenzenes. <i>Journal of Chemical Information and Computer Sciences</i> , 2002, 42, 284-289. | 2.8 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1238 | 1,8-Chalcogen-bridged naphthalenes. Strong carbon bases in the gas phase. <i>New Journal of Chemistry</i> , 2002, 26, 1747-1752. | 1.4 | 33 |
| 1239 | The formation of neutral CCC and its radical cation from the CCC radical anion in the gas phase. A joint experimental and theoretical study. <i>Perkin Transactions II RSC</i> , 2002, , 1647-1652. | 1.1 | 7 |
| 1240 | Theoretical Determination of Chromophores in the Chromogenic Effects of Aromatic Neurotoxicants. <i>Journal of the American Chemical Society</i> , 2002, 124, 2744-2752. | 6.6 | 38 |
| 1241 | From chelating to bridging diphosphine ligands in quadruply-bonded bimetallic complexes: a non-dissociative phosphine exchange mechanism. <i>New Journal of Chemistry</i> , 2002, 26, 1118-1121. | 1.4 | 6 |
| 1242 | Vibrational structure and vibronic coupling in the carbon 1s photoelectron spectra of benzene and deuterobenzene. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5937-5943. | 1.3 | 34 |
| 1243 | A hybrid quantum mechanical and empirical model for the prediction of isotropic ^{13}C shielding constants of organic molecules. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5498-5507. | 1.3 | 56 |
| 1244 | syn-Sesquinorbornenyl carbocations and their boron analogues: an ab initio and DFT study. <i>Perkin Transactions II RSC</i> , 2002, , 2057-2063. | 1.1 | 5 |
| 1245 | Influence of the variation of the co-ligands on the electronic transitions and emission properties of $[\text{Pt}(\text{I})(\text{CH}_3)_3(\text{iPr-DAB})]$, $[\text{Pt}(\text{CH}_3)_4(\pm\text{-diimine})]$ and $[\text{Pt}(\text{SnPh}_3)_2(\text{CH}_3)_2(\text{iPr-DAB})]$: an experimental and theoretical study. <i>Dalton Transactions RSC</i> , 2002, , 218-225. | 2.3 | 15 |
| 1246 | Theoretical enthalpies of formation of large compounds using integrated methods. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 4096-4102. | 1.3 | 11 |
| 1247 | Quantum-Chemical Methods for Accurate Theoretical Thermochemistry. , 2001, , 67-98. | | 1 |
| 1248 | The hydration structure of the lithium ion. <i>Journal of Chemical Physics</i> , 2002, 117, 110-117. | 1.2 | 133 |
| 1249 | On the Protonation Equilibrium for the Benzimidazole Derivative Hoechst 33258: An Electronic Molecular Orbital Study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2002, 20, 301-310. | 2.0 | 16 |
| 1250 | The Secret of Dimethyl Sulfoxide~Water Mixtures. A Quantum Chemical Study of $1\text{DMSO}\hat{\sim}\text{nWater}$ Clusters. <i>Journal of the American Chemical Society</i> , 2002, 124, 6206-6215. | 6.6 | 174 |
| 1251 | Density-functional theory of linear and nonlinear time-dependent molecular properties. <i>Journal of Chemical Physics</i> , 2002, 117, 9630-9645. | 1.2 | 359 |
| 1252 | $\text{TpPtMe}(\text{H})_2$: Why Is There H/D Scrambling of the Methyl Group but Not Methane Loss?. <i>Journal of the American Chemical Society</i> , 2002, 124, 7041-7054. | 6.6 | 63 |
| 1253 | The Reaction of Triplet Flavin with Indole. A Study of the Cascade of Reactive Intermediates Using Density Functional Theory and Time Resolved Infrared Spectroscopy. <i>Journal of the American Chemical Society</i> , 2002, 124, 7226-7234. | 6.6 | 108 |
| 1254 | Conformational Analysis Using Infrared and Vibrational Circular Dichroism Spectroscopies: The Chiral Cyclic Sulfoxides 1-Thiochroman-4-one-S-Oxide, 1-Thiaindan-S-Oxide and 1-Thiochroman-S-Oxide. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10510-10524. | 1.1 | 19 |
| 1255 | Anion~Aromatic Bonding: A Case for Anion Recognition by ~Acidic Rings. <i>Journal of the American Chemical Society</i> , 2002, 124, 6274-6276. | 6.6 | 598 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1256 | Asymmetric Weitzâ" Scheffer Epoxidation of Isoflavones with Hydroperoxides Mediated by Optically Active Phase-Transfer Catalysts. <i>Journal of Organic Chemistry</i> , 2002, 67, 259-264. | 1.7 | 73 |
| 1257 | The Photochemistry of Riboflavin Tetraacetate and Nucleosides. A Study Using Density Functional Theory, Laser Flash Photolysis, Fluorescence, UVâ"Vis, and Time Resolved Infrared Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2002, 106, 10263-10271. | 1.2 | 55 |
| 1258 | The Effect of Substituents on the Strain Energies of Small Ring Compounds. <i>Journal of Organic Chemistry</i> , 2002, 67, 2588-2599. | 1.7 | 67 |
| 1259 | The infrared spectra of C ₉ H ₁₂ O. <i>Journal of Physical Chemistry B</i> , 2002, 106, 10263-10271. | 1.6 | 52 |
| 1260 | Ab initio molecular orbital study of valence isomers of pyridine. <i>Computational and Theoretical Chemistry</i> , 2002, 578, 249-253. | 1.5 | 4 |
| 1261 | How accurately can we calculate molecular CH and CC re distances by DFT methods? Dependence on basis sets and functionals, estimations of experimentally inaccessible re distances and distance-dependent scaling factors for approximations of triple-zeta quality. <i>Computational and Theoretical Chemistry</i> , 2002, 578, 229-247. | 1.5 | 16 |
| 1263 | Synthese enantiomerenangereicherter 5-Alkyliden-2-cyclopentenone aus chiralen Allenylcarbamaten - Erzeugung chiraler Lithiumallenolate und allylische Aktivierung fÃ¼r die konrotatorische 4Î"Elektrocyclisierung. <i>Angewandte Chemie</i> , 2002, 114, 1610-1612. | 1.6 | 15 |
| 1265 | Sigmatropic Shiftamers: Fluxionality in Broken Ladderane Polymers. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 1033-1036. | 7.2 | 35 |
| 1266 | Synthesis of Enantioenriched 5-Alkylidene-2-cyclopentenones from Chiral Allenyl Carbamates: Generation of a Chiral Lithium Allenolate and Allylic Activation for a Conrotatory 4Î"Electrocyclization. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 1532-1535. | 7.2 | 48 |
| 1267 | Electronic Structure and Bonding in Hexacoordinate Silylâ"Palladium Complexes Support from the National Science Foundation (CHE-9876792) is gratefully acknowledged.. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 1953. | 7.2 | 36 |
| 1268 | Gas-Phase Detection of the Elusive Benzoborirene Molecule. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 2350-2352. | 7.2 | 24 |
| 1269 | A Novel Configuration of a Benzoylacetonato-Diorganotin Species is Modified by an Electron-Withdrawing Substituent on Tin â" Synthesis, IR and NMR Spectroscopy, Structure, and ab initio Studies. <i>European Journal of Inorganic Chemistry</i> , 2002, 2002, 1447-1455. | 1.0 | 11 |
| 1270 | Do Divalent [HC(CRâ"NRâ"â"2)E] Compounds Contain E(I) or E(III) (E = B, Al, Ga, In)? On the Correspondence of Formal Oxidation Numbers, Lewis Structures, and Reactivity. <i>European Journal of Inorganic Chemistry</i> , 2002, 2002, 1854-1863. | 1.0 | 24 |
| 1271 | Formation of Isomeric BAr ₃ Adducts of 2-Lithio-N-methylimidazole. <i>European Journal of Inorganic Chemistry</i> , 2002, 2002, 2015-2021. | 1.0 | 67 |
| 1272 | Mono and double polar [4 + 2+] Diels-Alder cycloaddition of acylium ions with O-heterodienes. <i>Journal of Mass Spectrometry</i> , 2002, 37, 146-154. | 0.7 | 17 |
| 1273 | Study of the temperature-dependent conformational averaging of ¹ H NMR resonances in vinylcyclopropane through the use of ab initio methodology and Boltzmann statistics. <i>Magnetic Resonance in Chemistry</i> , 2002, 40, 195-201. | 1.1 | 10 |
| 1274 | Determination of absolute configuration using vibrational circular dichroism spectroscopy: The chiral sulfoxide 1-thiochromanone S-oxide. <i>Chirality</i> , 2002, 14, 400-406. | 1.3 | 42 |
| 1275 | Absolute configuration and conformational analysis of a degradation product of inhalation anesthetic Sevoflurane: A vibrational circular dichroism study. <i>Chirality</i> , 2002, 14, 618-624. | 1.3 | 13 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1276 | Ab initio calculations for the optical rotations of conformationally flexible molecules: A case study on six-, seven-, and eight-membered fluorinated cycloalkanol esters. <i>Chirality</i> , 2002, 14, 793-797. | 1.3 | 69 |
| 1277 | Infrared and Quantum-Chemical Studies of Dimethylsilane. <i>Journal of Molecular Spectroscopy</i> , 2002, 216, 363-373. | 0.4 | 8 |
| 1278 | Ab initio conformational studies on diols and binary diol-water systems using DFT methods. Intramolecular hydrogen bonding and 1:1 complex formation with water. <i>Journal of Computational Chemistry</i> , 2002, 23, 585-599. | 1.5 | 104 |
| 1279 | Four-component relativistic Kohn-Sham theory. <i>Journal of Computational Chemistry</i> , 2002, 23, 814-823. | 1.5 | 147 |
| 1280 | A new molecular mechanics force field for the oxidized form of blue copper proteins. <i>Journal of Computational Chemistry</i> , 2002, 23, 697-705. | 1.5 | 79 |
| 1281 | Are allylic hydrogens in catechins more abstractable than catecholic hydrogens?. <i>JAOCS, Journal of the American Oil Chemists' Society</i> , 2002, 79, 943-944. | 0.8 | 14 |
| 1282 | Infrared spectra of two sexithiophenes in neutral and doped states: a theoretical and spectroscopic study. <i>Vibrational Spectroscopy</i> , 2002, 30, 175-189. | 1.2 | 7 |
| 1283 | Structural and vibrational study of the Ci(1) conformation of 18-crown-6. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2002, 58, 2877-2884. | 2.0 | 8 |
| 1284 | Small carbon clusters (C _n 0, C _n +, C _n âˆ“) from acyclic and cyclic precursors. <i>International Journal of Mass Spectrometry</i> , 2002, 217, 81-96. | 0.7 | 26 |
| 1285 | Adducts of NF ₂ + with diatomic and simple polyatomic ligands: a computational investigation on the structure, stability, and thermochemistry. <i>International Journal of Mass Spectrometry</i> , 2002, 216, 285-299. | 0.7 | 24 |
| 1286 | Experimental and theoretical studies on the gas phase reactivity of formamideâ€™Ni+ complexes generated by FAB and electrospray ionization. <i>International Journal of Mass Spectrometry</i> , 2002, 219, 429-443. | 0.7 | 9 |
| 1287 | Towards the characterization of the mechanism of the sequential activation of four methane molecules by Ta+. <i>International Journal of Mass Spectrometry</i> , 2002, 219, 457-473. | 0.7 | 20 |
| 1288 | The performance of density function theory in describing gas-phase SN ₂ reactions at saturated nitrogen. <i>International Journal of Mass Spectrometry</i> , 2002, 221, 59-65. | 0.7 | 26 |
| 1289 | The challenges of combustion for chemical theory. <i>Proceedings of the Combustion Institute</i> , 2002, 29, 1173-1200. | 2.4 | 22 |
| 1290 | Reaction mechanism of thymine dimer formation in DNA induced by UV light. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2002, 152, 95-101. | 2.0 | 80 |
| 1291 | Generation and characterization of ionic and neutral P(OH) ₂ +/. in the gas phase by tandem mass spectrometry and computational chemistry. <i>Journal of the American Society for Mass Spectrometry</i> , 2002, 13, 250-264. | 1.2 | 11 |
| 1292 | Reliability of ab initio (HF, post HF and DFT) methods and basis set dependencies for accurate prediction of equilibrium r e distances of CO bond lengths. <i>Computational and Theoretical Chemistry</i> , 2002, 585, 35-47. | 1.5 | 11 |
| 1293 | Long-range substituent influence on the equatorial/axial conformational equilibrium of cyclohexanol and cyclohexanthiol esters. <i>Computational and Theoretical Chemistry</i> , 2002, 585, 223-237. | 1.5 | 14 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1294 | Reactions of oxiranylidene and dimethyloxiranylidene, and their generation by retro Diels-Alder-type reactions: a computational study. <i>Computational and Theoretical Chemistry</i> , 2002, 593, 79-91. | 1.5 | 6 |
| 1295 | Effect of coordinated water on the mechanism of neutral hydrolysis of silicon dioxide in gas phase: a first principles study. <i>Computational and Theoretical Chemistry</i> , 2002, 592, 53-60. | 1.5 | 2 |
| 1296 | Computational probes into the conceptual basis of silver ion chromatography: I. Silver(I) ion complexes of unsaturated fatty acids and esters. <i>Computational and Theoretical Chemistry</i> , 2002, 589-590, 239-249. | 1.5 | 21 |
| 1297 | Evaluation of the effectiveness of AM1 geometry used in calculating O-H bond dissociation enthalpy. <i>Computational and Theoretical Chemistry</i> , 2002, 618, 181-189. | 1.5 | 8 |
| 1298 | Valence orbital electron momentum distributions for dimethylsulfide: comparison of EMS measurements with near Hartree-Fock limit and density functional theory calculations. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2002, 123, 377-388. | 0.8 | 10 |
| 1299 | Synthesis, X-ray crystal structure and solution behaviour of $[Zn\{\eta^5-C_5H_5\}Fe\{\eta^5-C_5H_4\}\eta^1-CH_3\eta^1-Ni\eta^1-(CH_2)_3\eta^1-NMe_2\}Cl_2]$. <i>Polyhedron</i> , 2002, 21, 2361-2367. | 1.0 | 4 |
| 1300 | Theoretical study of amino acid precursor formation in the interstellar medium. 2. Reaction of methylenimine with CN radical. <i>Advances in Space Research</i> , 2002, 30, 1445-1450. | 1.2 | 8 |
| 1301 | Theoretical study of amino acid precursor formation in the interstellar medium. 1. Reaction of methylenimine with hydrogen cyanide. <i>Advances in Space Research</i> , 2002, 30, 1439-1444. | 1.2 | 7 |
| 1302 | Mechanism and dynamics of organic reactions: 1,2-H shift in methylchlorocarbene. <i>Journal of Physical Organic Chemistry</i> , 2002, 15, 431-447. | 0.9 | 28 |
| 1303 | Computational determination of the enthalpic and entropic contributions to the conformational preference of monosubstituted cyclohexanes. Molecular mechanics, semiempirical and density functional theory methods and ab initio calculations. <i>Journal of Physical Organic Chemistry</i> , 2002, 15, 808-819. | 0.9 | 7 |
| 1304 | Adiabatic connection method for $X^{\ddagger}+RX$ nucleophilic substitution reactions ($X^{\ddagger}=F, Cl$). <i>Journal of Physical Organic Chemistry</i> , 2002, 15, 712-720. | 0.9 | 34 |
| 1305 | Density functional study on geometry and electronic structure of nitrile hydratase active site model. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 1174-1187. | 1.0 | 13 |
| 1306 | Quadricyclane radical cation isomerization reactions: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 1388-1395. | 1.0 | 9 |
| 1307 | Superacid catalyzed reactions of 5-amino-1-naphthol with benzene and cyclohexane. <i>Tetrahedron</i> , 2002, 58, 5423-5426. | 1.0 | 32 |
| 1308 | The NMR shifts are not a measure for the nakedness of the fluoride anion. <i>Journal of Fluorine Chemistry</i> , 2002, 116, 49-58. | 0.9 | 57 |
| 1309 | Ab initio and DFT calculations of the structure and vibrational spectra of trigonelline. <i>Journal of Molecular Structure</i> , 2002, 614, 97-108. | 1.8 | 29 |
| 1310 | Molecular structures of trimeric diphenyltin chalcogenides, $(Ph_2SnE)_3$, E=S, Se, Te. <i>Journal of Organometallic Chemistry</i> , 2002, 660, 43-49. | 0.8 | 20 |
| 1311 | Thermal decomposition of energetic materials. <i>Thermochimica Acta</i> , 2002, 388, 227-232. | 1.2 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1312 | Spin- ρ spin coupling tensors as determined by experiment and computational chemistry. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2002, 41, 233-304. | 3.9 | 169 |
| 1313 | On the evaluation of thermal corrections to gas phase ab initio relative energies: implications to the conformational analysis study of cyclooctane. <i>Chemical Physics</i> , 2002, 280, 31-42. | 0.9 | 35 |
| 1314 | DFT calculation on the energy thresholds of DNA damages under irradiation conditions. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2002, 300, 421-426. | 0.9 | 6 |
| 1315 | Prediction and interpretation of the ^{57}Fe isomer shift in Mössbauer spectra by density functional theory. <i>Inorganica Chimica Acta</i> , 2002, 337, 181-192. | 1.2 | 547 |
| 1316 | Ligand-to-ligand charge transfer states and photochemical bond homolysis in metal-carbon bonded platinum complexes. <i>Coordination Chemistry Reviews</i> , 2002, 230, 193-211. | 9.5 | 61 |
| 1317 | The vibrations of benzene, studied by 'Multimode'. <i>Chemical Physics Letters</i> , 2002, 354, 1-8. | 1.2 | 21 |
| 1318 | A new quasi-relativistic approach for density functional theory based on the normalized elimination of the small component. <i>Chemical Physics Letters</i> , 2002, 351, 259-266. | 1.2 | 30 |
| 1319 | An ab initio study of the equilibrium geometry and vibrational frequencies of hydrazine. <i>Chemical Physics Letters</i> , 2002, 352, 120-126. | 1.2 | 28 |
| 1320 | The role of frontier molecular orbital ordering on electronic communication in porphyrin arrays. <i>Chemical Physics Letters</i> , 2002, 353, 111-118. | 1.2 | 27 |
| 1321 | Optical rotation studied by density-functional and coupled-cluster methods. <i>Chemical Physics Letters</i> , 2002, 352, 533-539. | 1.2 | 192 |
| 1322 | A Kohn-Sham study of the oxirene-ketene potential energy surface. <i>Chemical Physics Letters</i> , 2002, 352, 540-544. | 1.2 | 16 |
| 1323 | Ab initio calculations predict a very low barrier for the rotation of the axial ligand in $\text{Fe}(\text{P})(\text{Im})$. <i>Chemical Physics Letters</i> , 2002, 353, 379-382. | 1.2 | 10 |
| 1325 | Parity-violating interaction in H_2O_2 calculated from density-functional theory. <i>Chemical Physics Letters</i> , 2002, 354, 274-282. | 1.2 | 44 |
| 1326 | Adsorption energy surfaces in faujasite type zeolites. <i>Chemical Physics Letters</i> , 2002, 354, 474-482. | 1.2 | 12 |
| 1327 | Mechanisms for the growth of polycyclic aromatic hydrocarbon (PAH) cations. <i>Chemical Physics Letters</i> , 2002, 355, 159-163. | 1.2 | 19 |
| 1328 | Theoretical study of C_{20} fullerene dimerization: a facile [2+2] cycloaddition. <i>Chemical Physics Letters</i> , 2002, 359, 446-452. | 1.2 | 22 |
| 1329 | Diatomic bond lengths and vibrational frequencies: assessment of recently developed exchange-correlation functionals. <i>Chemical Physics Letters</i> , 2002, 360, 38-46. | 1.2 | 34 |
| 1330 | Obtaining the right orbitals is the first step to calculating accurate binding energies for Cu^+ ion. <i>Chemical Physics Letters</i> , 2002, 361, 251-258. | 1.2 | 23 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1331 | An improved method for density functional calculations of the frequency-dependent optical rotation. <i>Chemical Physics Letters</i> , 2002, 361, 321-328. | 1.2 | 189 |
| 1332 | A study of the isomers of C ₃₆ fullerene using single and multireference MP2 perturbation theory. <i>Chemical Physics Letters</i> , 2002, 362, 380-386. | 1.2 | 20 |
| 1333 | Energy density analysis with Kohn-Sham orbitals. <i>Chemical Physics Letters</i> , 2002, 363, 73-79. | 1.2 | 126 |
| 1334 | Synthesis, crystal structure and magnetic properties of a novel nitroxide biradical. Theoretical investigation of the exchange mechanisms. <i>Chemical Physics Letters</i> , 2002, 364, 393-401. | 1.2 | 32 |
| 1335 | Dipole moments in excited state DFT calculations. <i>Chemical Physics Letters</i> , 2002, 364, 612-615. | 1.2 | 27 |
| 1336 | Energy density analysis (EDA) of cis, trans-enol isomerization in malonaldehyde, tropolone and 9-hydroxyphenalenone. <i>Chemical Physics Letters</i> , 2002, 365, 203-210. | 1.2 | 27 |
| 1337 | Theoretical Analysis of CO Adsorption on the Reduced Cr/Silica System. <i>Journal of Catalysis</i> , 2002, 205, 177-190. | 3.1 | 32 |
| 1338 | Silver Ion Binding Energies of Amino Acids: Use of Theory to Assess the Validity of Experimental Silver Ion Basicities Obtained from the Kinetic Method. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6121-6128. | 1.1 | 141 |
| 1339 | Reduced and Excited States of (bpym)[PtCl ₂] _n (bpym = 2,2'-Bipyrimidine; n = 1, 2): Experiments and DFT Calculations. <i>Inorganic Chemistry</i> , 2002, 41, 4139-4148. | 1.9 | 39 |
| 1340 | High Coverages of Hydrogen on (10,0), (9,0) and (5,5) Carbon Nanotubes. <i>Nano Letters</i> , 2002, 2, 337-341. | 4.5 | 64 |
| 1341 | Sulfur-Gold Orbital Interactions which Determine the Structure of Alkanethiolate/Au(111) Self-Assembled Monolayer Systems. <i>Journal of Physical Chemistry B</i> , 2002, 106, 12727-12736. | 1.2 | 135 |
| 1342 | Model Calculations of Radiation-Induced Damage in 1-Methyluracil:9-Ethyladenine. <i>Structural Chemistry</i> , 2002, 13, 203-209. | 1.0 | 4 |
| 1343 | Theoretical Elucidation on the Antioxidant Mechanism of Curcumin: A DFT Study. <i>Organic Letters</i> , 2002, 4, 2909-2911. | 2.4 | 159 |
| 1344 | Cycloaddition Reactions of Metalloaromatic Complexes of Iridium and Rhodium: A Mechanistic DFT Investigation. <i>Journal of the American Chemical Society</i> , 2003, 125, 11702-11709. | 6.6 | 53 |
| 1345 | A Standard Set of Pericyclic Reactions of Hydrocarbons for the Benchmarking of Computational Methods: The Performance of ab Initio, Density Functional, CASSCF, CASPT2, and CBS-QB3 Methods for the Prediction of Activation Barriers, Reaction Energetics, and Transition State Geometries. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11445-11459. | 1.1 | 342 |
| 1346 | Steric and Electronic Structure of C ₆ H ₅ XCF ₃ Molecules (X = O or S): A Quantum-Chemical Study. <i>Russian Journal of General Chemistry</i> , 2003, 73, 229-239. | 0.3 | 4 |
| 1347 | Five-, six- and eight-membered ring organosilicon chalcogenides of the types Z ₂ (SiMe ₂) ₂ E (Z = Me ₂ Si, E = S, Se). <i>Silicon Chemistry</i> , 2003, 2, 77-92. | 0.8 | 40 |
| 1348 | A DFT and MP2 Study on the Molecular Structure and Vibrational Spectra of Halogenosubstituted Phosphoryl and Thiophosphoryl Compounds. <i>Structural Chemistry</i> , 2003, 14, 511-525. | 1.0 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1349 | Intramolecular Reactions of Alkynes with Furans and Electron Rich Arenes Catalyzed by PtCl ₂ : The Role of Platinum Carbenes as Intermediates. <i>Journal of the American Chemical Society</i> , 2003, 125, 5757-5766. | 6.6 | 260 |
| 1350 | Improved second-order Møller-Plesset perturbation theory by separate scaling of parallel- and antiparallel-spin pair correlation energies. <i>Journal of Chemical Physics</i> , 2003, 118, 9095-9102. | 1.2 | 1,607 |
| 1351 | Alkane Oxidation by VO ₂ in the Gas Phase: A Unique Dependence of Reactivity on the Chain Length. <i>Organometallics</i> , 2003, 22, 3933-3943. | 1.1 | 67 |
| 1352 | Hydrogen Atom Adducts to the Amide Bond. Generation and Energetics of Amide Radicals in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2003, 107, 115-126. | 1.1 | 73 |
| 1353 | Reactions of Laser-Ablated Chromium Atoms, Cations, and Electrons with CO in Excess Argon and Neon: Infrared Spectra and Density Functional Calculations on Neutral and Charged Unsaturated Chromium Carbonyls. <i>Journal of Physical Chemistry A</i> , 2003, 107, 561-569. | 1.1 | 30 |
| 1354 | Ab Initio Calculations for Hydrocarbons: Enthalpy of Formation, Transition State Geometry, and Activation Energy for Radical Reactions. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9147-9159. | 1.1 | 170 |
| 1355 | Infrared Spectra of Group 14 Hydrides in Solid Hydrogen: Experimental Observation of PbH ₄ , Pb ₂ H ₂ , and Pb ₂ H ₄ . <i>Journal of the American Chemical Society</i> , 2003, 125, 6581-6587. | 6.6 | 98 |
| 1356 | A theoretical investigation on DPPH radical-Scavenging mechanism of edaravone. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2003, 13, 3789-3792. | 1.0 | 63 |
| 1357 | Allyl stannanes as electrophiles or nucleophiles in the palladium-catalyzed reactions with alkynes. <i>Journal of Organometallic Chemistry</i> , 2003, 687, 410-419. | 0.8 | 27 |
| 1358 | Calculated structures of [Au=C=Au] ²⁺ and related systems. <i>Chemical Physics Letters</i> , 2003, 381, 45-52. | 1.2 | 45 |
| 1359 | Does the radical Me ₃ O exist in the gas phase? A joint experimental and theoretical study. <i>International Journal of Mass Spectrometry</i> , 2003, 230, 77-83. | 0.7 | 3 |
| 1360 | Accuracy assessment of semiempirical molecular electrostatic potential of proteins. <i>Theoretical Chemistry Accounts</i> , 2003, 109, 213-219. | 0.5 | 4 |
| 1361 | Towards a "next generation" neglect of diatomic differential overlap based semiempirical molecular orbital technique. <i>Theoretical Chemistry Accounts</i> , 2003, 110, 254-266. | 0.5 | 64 |
| 1362 | Catalysis by methyl-coenzyme M reductase: a theoretical study for heterodisulfide product formation. <i>Journal of Biological Inorganic Chemistry</i> , 2003, 8, 653-662. | 1.1 | 70 |
| 1363 | AM1* parameters for phosphorus, sulfur and chlorine. <i>Journal of Molecular Modeling</i> , 2003, 9, 408-414. | 0.8 | 74 |
| 1364 | Optimal Spectrum Estimation in Statistical Mechanics. <i>ChemPhysChem</i> , 2003, 4, 1227-1230. | 1.0 | 20 |
| 1365 | Accurate Quantum-Chemical Prediction of Enthalpies of Formation of Small Molecules in the Gas Phase. <i>ChemPhysChem</i> , 2003, 4, 32-48. | 1.0 | 41 |
| 1366 | Substantial Errors from Time-Dependent Density Functional Theory for the Calculation of Excited States of Large π Systems. <i>ChemPhysChem</i> , 2003, 4, 292-295. | 1.0 | 463 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1367 | Quasiharmonic Vibrations of Water, Water Dimer, and Liquid Water from Principal Component Analysis of Quantum or QM/MM Trajectories. <i>ChemPhysChem</i> , 2003, 4, 382-384. | 1.0 | 37 |
| 1368 | Interactions of Atomic Iron Cation with Pyridine and Benzene: A Theoretical Study on an Unresolved Controversy of Bond Energies and Electronic Ground-State Structures. <i>Helvetica Chimica Acta</i> , 2003, 86, 1008-1025. | 1.0 | 13 |
| 1369 | An Unexpected Atropisomerically Stable 1,1-Biphenyl at Ambient Temperature in Solution, Elucidated by Vibrational Circular Dichroism (VCD). <i>Helvetica Chimica Acta</i> , 2003, 86, 3141-3155. | 1.0 | 19 |
| 1370 | Helicoid Shiftamers for the Transport of π -Clumps and Charges. <i>Helvetica Chimica Acta</i> , 2003, 86, 3525-3532. | 1.0 | 9 |
| 1371 | Fast approximate methods for calculating nucleic acid base pair interaction energies. <i>Journal of Computational Chemistry</i> , 2003, 24, 57-67. | 1.5 | 30 |
| 1372 | Parameterization of charge model 3 for AM1, PM3, BLYP, and B3LYP. <i>Journal of Computational Chemistry</i> , 2003, 24, 1291-1304. | 1.5 | 107 |
| 1373 | Hydrogen bonding in diols and binary diol-water systems investigated using DFT methods. II. Calculated infrared OH-stretch frequencies, force constants, and NMR chemical shifts correlate with hydrogen bond geometry and electron density topology. A reevaluation of geometrical criteria for hydrogen bonding. <i>Journal of Computational Chemistry</i> , 2003, 24, 1120-1131. | 1.5 | 79 |
| 1374 | Improved third-order Møller-Plesset perturbation theory. <i>Journal of Computational Chemistry</i> , 2003, 24, 1529-1537. | 1.5 | 117 |
| 1375 | Reassessment of methyl rotation barriers and conformations by correlated quantum chemistry methods. <i>Journal of Computational Chemistry</i> , 2003, 24, 2093-2100. | 1.5 | 16 |
| 1376 | Structural Characterization and a New One-Pot Synthesis of trans-Chloro(phenyl)bis(triphenylphosphane)nickel(II). <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 1802-1806. | 1.0 | 43 |
| 1377 | Co-Ligand Involvement in Ground and Excited States of Electron-Rich (Polypyridyl)Pt(II) Complexes. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 1917-1938. | 1.0 | 32 |
| 1378 | (4-Acyl-5-pyrazolonato)titanium Derivatives: Oligomerization, Hydrolysis, Voltammetry, and DFT Study. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 3221-3232. | 1.0 | 51 |
| 1379 | Synthesis and Reactivity of the First σ -6-Rhodium(I) and σ -6-Iridium(I) Complexes of 2,6-Bis(trimethylsilyl)phosphinines. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 687-698. | 1.0 | 38 |
| 1380 | Manganese-Salen Complexes as Oxygen-Transfer Agents in Catalytic Epoxidations \hat{a} A Density Functional Study of Mechanistic Aspects. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 892-902. | 1.0 | 69 |
| 1381 | Chelate Complexes of Functionalized Cycloheptatrienyl Ligands: Molybdenum Complexes with Linked Cycloheptatrienyl-Phosphane Ligands and Their Use in Catalytic Carbon \hat{a} Carbon Bond Formation. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 1088-1098. | 1.0 | 23 |
| 1382 | A DFT Study of Tin- and Crown-Ether-Based Host Molecules Capable of Binding Anions and Cations Simultaneously. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 1315-1324. | 1.0 | 21 |
| 1383 | Structures of Carbonato and Bicarbonato Complexes of Bis(1,10-phenanthroline)Zinc(II): Experiment and Theory. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 1562-1569. | 1.0 | 15 |
| 1384 | Cyclisation of Novel Amino Oxo Esters to Tetramic Acids \hat{a} Density Functional Theory Study of the Reaction Mechanism. <i>European Journal of Organic Chemistry</i> , 2003, 2003, 4593-4600. | 1.2 | 9 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1385 | Diradical versus Concerted Mechanisms for the Dihydroxylation of Protoanemonin by OsO ₄ and OsO ₄ ·NH ₃ · The Effect of the Base in the Reaction. <i>European Journal of Organic Chemistry</i> , 2003, 2003, 833-839. | 1.2 | 8 |
| 1386 | Peptide cation-radicals. A computational study of the competition between peptide N-C bond cleavage and loss of the side chain in the [GlyPhe-NH ₂ + 2H] ⁺ cation-radical. <i>Journal of Mass Spectrometry</i> , 2003, 38, 1093-1104. | 0.7 | 48 |
| 1387 | Carbon Tetraoxide: Theoretically Predicted and Experimentally Detected. <i>Angewandte Chemie</i> , 2003, 115, 3093-3098. | 1.6 | 4 |
| 1388 | Stereoelectronic, Strain, and Medium Effects on the Protonation of Cubylamine, a Janus-like Base. <i>Angewandte Chemie</i> , 2003, 115, 2383-2387. | 1.6 | 3 |
| 1392 | Protonation of Cubane in the Gas Phase: A High-Level Ab Initio and DFT Study. <i>Angewandte Chemie</i> , 2003, 115, 1074-1076. | 1.6 | 6 |
| 1393 | Absolute configuration determination of chiral molecules in the solution state using vibrational circular dichroism. <i>Chirality</i> , 2003, 15, 743-758. | 1.3 | 483 |
| 1394 | A Non-Radical Mechanism for Methane Hydroxylation at the Diiron Active Site of Soluble Methane Monooxygenase. <i>Chemistry - A European Journal</i> , 2003, 9, 2347-2358. | 1.7 | 40 |
| 1395 | On the Electronic Structures of the 1,3-Diboracyclobutane-1,3-diyls and Their Valence Isomers with a B ₂ E ₂ Skeleton (E=N, P, As). <i>Chemistry - A European Journal</i> , 2003, 9, 3611-3617. | 1.7 | 53 |
| 1396 | Vibrational and Quantum-Chemical Study of Push-Pull Chromophores for Second-Order Nonlinear Optics from Rigidified Thiophene-Based π -Conjugating Spacers. <i>Chemistry - A European Journal</i> , 2003, 9, 3670-3682. | 1.7 | 57 |
| 1397 | Mechanism of Aromatic Hydroxylation by an Activated Fe/V $\frac{3}{4}$ O Core in Tetrahydrobiopterin-Dependent Hydroxylases. <i>Chemistry - A European Journal</i> , 2003, 9, 4055-4067. | 1.7 | 69 |
| 1398 | Resonance-Assisted Intramolecular Chalcogen-Chalcogen Interactions?. <i>Chemistry - A European Journal</i> , 2003, 9, 4548-4555. | 1.7 | 79 |
| 1399 | Mechanism of Dioxygen Cleavage in Tetrahydrobiopterin-Dependent Amino Acid Hydroxylases. <i>Chemistry - A European Journal</i> , 2003, 9, 106-115. | 1.7 | 63 |
| 1400 | A Comprehensive Theoretical Study on the Reactions of Sc ⁺ with C _n H _{2n+2} (n=1-3): Structure, Mechanism, and Potential-Energy Surface. <i>Chemistry - A European Journal</i> , 2003, 9, 484-501. | 1.7 | 33 |
| 1401 | Substituent Effects on O-H Bond Dissociation Enthalpies and Ionization Potentials of Catechols: A DFT Study and Its Implications in the Rational Design of Phenolic Antioxidants and Elucidation of Structure-Activity Relationships for Flavonoid Antioxidants. <i>Chemistry - A European Journal</i> , 2003, 9, 502-508. | 1.7 | 204 |
| 1402 | Carbon Tetraoxide: Theoretically Predicted and Experimentally Detected. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 2985-2990. | 7.2 | 15 |
| 1403 | Stereoelectronic, Strain, and Medium Effects on the Protonation of Cubylamine, a Janus-like Base. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 2281-2285. | 7.2 | 18 |
| 1404 | Polyhedral Boranes with Exo Multiple Bonds: Three-Dimensional Inorganic Analogues of Quinones. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 3777-3781. | 7.2 | 12 |
| 1405 | Polyazide Chemistry: Preparation and Characterization of Te(N ₃) ₄ and [P(C ₆ H ₅) ₄] ₂ [Te(N ₃) ₆] and Evidence for [N(CH ₃) ₄][Te(N ₃) ₅]. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 5847-5851. | 7.2 | 91 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1406 | Breaking Down Barriers: The Liaison Between Sigmatropic Shifts, Electrocyclic Reactions, and Three-Center Cations. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 5877-5882. | 7.2 | 20 |
| 1407 | Protonation of Cubane in the Gas Phase: A High-Level Ab Initio and DFT Study. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 1044-1046. | 7.2 | 17 |
| 1408 | Condensed polyhedral boranes and analogous organometallic clusters: a molecular orbital and density functional theory study on the cap-cap interactions. <i>Applied Organometallic Chemistry</i> , 2003, 17, 480-492. | 1.7 | 10 |
| 1409 | Numerical simulations of Raman spectra of guanine-cytosine Watson-Crick and protonated Hoogsteen base pairs. <i>Biopolymers</i> , 2003, 72, 339-344. | 1.2 | 15 |
| 1410 | Sulfur hexafluoride corona discharge decomposition: gas-phase ion chemistry of SOF ⁺ (x=1-3) ions. <i>Chemical Physics Letters</i> , 2003, 381, 168-176. | 1.2 | 14 |
| 1411 | Modelling of benzene-1,4-dithiol on a Au(111) surface. <i>Chemical Physics Letters</i> , 2003, 367, 90-94. | 1.2 | 23 |
| 1412 | Geometries and electronic properties of Au _n Pd _m (n=1-4, m=1, 0, 1) clusters. <i>Chemical Physics Letters</i> , 2003, 368, 153-161. | 1.2 | 24 |
| 1413 | Energy density analysis of internal methyl rotations in halogenated toluenes. <i>Chemical Physics Letters</i> , 2003, 368, 673-679. | 1.2 | 22 |
| 1414 | Ab initio correlated comparative study of the torsional potentials for 2,2'-bipyrrrole and 2,2'-bifuran five membered heterocyclic dimers. <i>Chemical Physics Letters</i> , 2003, 369, 114-124. | 1.2 | 24 |
| 1415 | Conductivity at low temperatures, are the rings eclipsed or perpendicular?. <i>Chemical Physics Letters</i> , 2003, 369, 415-418. | 1.2 | 3 |
| 1416 | Relativistically corrected geometries obtained with analytical gradients: normalized elimination of the small component using an effective potential. <i>Chemical Physics Letters</i> , 2003, 370, 647-653. | 1.2 | 17 |
| 1417 | Potential energy surface of aluminum and tungsten dimers. <i>Chemical Physics Letters</i> , 2003, 371, 35-39. | 1.2 | 11 |
| 1418 | Sternheimer shieldings and EFG polarizabilities: a density-functional theory study. <i>Chemical Physics Letters</i> , 2003, 372, 377-385. | 1.2 | 4 |
| 1419 | Reactions of HOBr + HCl + nH ₂ O and HOBr + HBr + nH ₂ O. <i>Chemical Physics Letters</i> , 2003, 372, 569-576. | 1.2 | 7 |
| 1420 | Calculations of hydrogen-bond-transmitted indirect nuclear spin-spin couplings: a comparison of density-functional and ab initio methods. <i>Chemical Physics Letters</i> , 2003, 372, 476-484. | 1.2 | 27 |
| 1421 | On the current flow for benzene-1,4-dithiol between two Au contacts. <i>Chemical Physics Letters</i> , 2003, 372, 723-727. | 1.2 | 19 |
| 1422 | Interaction of a conjugated phenylene ethynylene trimer with a Au(111) surface. <i>Chemical Physics Letters</i> , 2003, 372, 873-877. | 1.2 | 16 |
| 1423 | Theoretical enthalpy of formation of the acetyl radical. <i>Chemical Physics Letters</i> , 2003, 373, 350-356. | 1.2 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1424 | Calculations of two-photon absorption cross sections by means of density-functional theory. <i>Chemical Physics Letters</i> , 2003, 374, 446-452. | 1.2 | 136 |
| 1425 | Theoretical study of role of H ₂ O molecule on initial stage of reduction of O ₂ molecule in active site of cytochrome c oxidase. <i>Chemical Physics Letters</i> , 2003, 374, 45-52. | 1.2 | 24 |
| 1426 | Model calculations of the electron affinities and ionization potentials of DNA. <i>Chemical Physics Letters</i> , 2003, 374, 496-500. | 1.2 | 28 |
| 1427 | On the reaction of N and O atoms with carbon nanotubes. <i>Chemical Physics Letters</i> , 2003, 374, 501-505. | 1.2 | 30 |
| 1428 | On the bathochromic shift of the absorption by astaxanthin in crustacyanin: a quantum chemical study. <i>Chemical Physics Letters</i> , 2003, 375, 30-38. | 1.2 | 42 |
| 1429 | H+H ₂ quantum dynamics using potential energy surfaces from density functional theory. <i>Chemical Physics Letters</i> , 2003, 375, 162-166. | 1.2 | 8 |
| 1430 | Do individual molecule rotational barriers explain the retention times of molecular memories?. <i>Chemical Physics Letters</i> , 2003, 375, 459-462. | 1.2 | 9 |
| 1431 | Calculation of the gas phase specific rotation of (S)-propylene oxide at 355 nm. <i>Chemical Physics Letters</i> , 2003, 376, 452-456. | 1.2 | 45 |
| 1432 | Reactions of protonated water clusters H ⁺ (H ₂ O) _n (n=1-6) with dimethylsulfoxide in a guided ion beam apparatus. <i>Chemical Physics Letters</i> , 2003, 377, 69-73. | 1.2 | 41 |
| 1433 | Theoretical enthalpies of formation and C-H bond dissociation enthalpies of n-bromopropane and its free radicals. <i>Chemical Physics Letters</i> , 2003, 377, 607-612. | 1.2 | 5 |
| 1434 | Modeling the spin-dependent properties of open-shell Fe(III)-containing systems: towards a computational description of nitrile hydratase. <i>Coordination Chemistry Reviews</i> , 2003, 238-239, 291-314. | 9.5 | 32 |
| 1435 | Towards a rigorously defined quantum chemical analysis of the chemical bond in donor-acceptor complexes. <i>Coordination Chemistry Reviews</i> , 2003, 238-239, 55-82. | 9.5 | 394 |
| 1436 | S-H proton dissociation enthalpies of thiophenolic cation radicals: a DFT study. <i>Computational and Theoretical Chemistry</i> , 2003, 663, 167-174. | 1.5 | 42 |
| 1437 | Molecular structure and vibrational spectra of 4-tert-butylpyridine by density functional theory and ab initio Hartree-Fock calculations. <i>Computational and Theoretical Chemistry</i> , 2003, 663, 127-134. | 1.5 | 5 |
| 1438 | A multi-configurational study of the one-dimensional dissociation of azidopentazole (N ₈) and derived N ₇ CH isomers. <i>Computational and Theoretical Chemistry</i> , 2003, 663, 135-143. | 1.5 | 11 |
| 1439 | The role of submicrometer aerosols and macromolecules in H ₂ formation in the titan haze. <i>Icarus</i> , 2003, 161, 468-473. | 1.1 | 14 |
| 1440 | DFT studies of structures and enatiomerization mechanisms of bis-chelate complexes of Group 12 elements. <i>Inorganica Chimica Acta</i> , 2003, 353, 15-21. | 1.2 | 16 |
| 1441 | Surface to bulk charge transfer at an alkali metal/metal oxide interface. <i>Surface Science</i> , 2003, 547, L859-L864. | 0.8 | 22 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1442 | Helicity of N,N-dialkyl-trans-1,2-diaminocyclohexane derivatives. Implications for molecular helicity manipulations. <i>Tetrahedron</i> , 2003, 59, 9323-9331. | 1.0 | 16 |
| 1443 | Synthesis, molecular structure, and chemical reactivity of azuleno[1,2-a]acenaphthylene. <i>Tetrahedron</i> , 2003, 59, 801-811. | 1.0 | 4 |
| 1444 | Structural and vibrational properties of trigonellinium perchlorate dimer, (TRGH ⁺ ClO ₄) ₂ . <i>Journal of Molecular Structure</i> , 2003, 649, 43-53. | 1.8 | 3 |
| 1445 | Vibrational spectroscopy using ab initio density-functional techniques. <i>Journal of Molecular Structure</i> , 2003, 651-653, 3-17. | 1.8 | 27 |
| 1446 | Theoretical description of the Raman spectrum of a vinylene-bridged quaterthiophene oligomer. <i>Journal of Molecular Structure</i> , 2003, 651-653, 657-664. | 1.8 | 9 |
| 1447 | X-ray and B3LYP structures and vibrational spectra of pyridine betaine perchlorate monohydrate and conformation of a %N+CH ₂ COO moiety in crystalline betaines. <i>Journal of Molecular Structure</i> , 2003, 651-653, 621-634. | 1.8 | 21 |
| 1448 | Density functional IR, Raman, and VCD spectra of halogen substituted $\hat{1}^2$ -lactams. <i>Journal of Molecular Structure</i> , 2003, 651-653, 705-717. | 1.8 | 13 |
| 1449 | Molecular structure and vibrational spectra of 1,2-bis(4-pyridyl) ethane by density functional theory and ab initio Hartree-Fock calculations. <i>Journal of Molecular Structure</i> , 2003, 654, 1-9. | 1.8 | 45 |
| 1450 | Azo compounds as electron acceptor or radical ligands in transition metal species: spectroelectrochemistry and high-field EPR studies of ruthenium, rhodium and copper complexes of 2,2-azobis(5-chloropyrimidine). <i>Journal of Molecular Structure</i> , 2003, 656, 183-194. | 1.8 | 25 |
| 1451 | Crystal and single molecule structures of N-(carbomethoxymethyl)-pyridinium perchlorate. <i>Journal of Molecular Structure</i> , 2003, 657, 125-136. | 1.8 | 1 |
| 1452 | CO adsorption on MgO() surface with oxygen vacancy and its low-coordinated surface sites: embedded cluster model density functional study employing charge self-consistent technique. <i>Surface Science</i> , 2003, 525, 13-23. | 0.8 | 54 |
| 1453 | A DFT study of the magnetic properties and the iron-iron interaction in the Cp ₂ Fe ₂ ($\hat{1}^1/4$ S ₂ , $\hat{1}^2/4$ S ₂) and Cp ₂ Fe ₂ ($\hat{1}^2/4$ S ₂ , $\hat{1}^1/4$ S ₂) ₂ isomers of the Cp ₂ Fe ₂ S ₄ complex. <i>Computational and Theoretical Chemistry</i> , 2003, 1.5 621, 113-118. | 1.5 | 2 |
| 1454 | Flavin reduction potential tuning by substitution and bending. <i>Computational and Theoretical Chemistry</i> , 2003, 623, 185-195. | 1.5 | 51 |
| 1455 | Theoretical study on the isomerization of peroxyxynitrous acid (HOONO). <i>Computational and Theoretical Chemistry</i> , 2003, 624, 115-121. | 1.5 | 10 |
| 1456 | A way to compare experimental and SCRF electronic static dipole polarizability of pure liquids. <i>Computational and Theoretical Chemistry</i> , 2003, 630, 1-9. | 1.5 | 7 |
| 1457 | Electronic spectrum of Co-corrin calculated with the TDDFT method. <i>Computational and Theoretical Chemistry</i> , 2003, 631, 209-223. | 1.5 | 26 |
| 1458 | Theoretical assessment on the viability of possible intermediates in the reaction mechanism of catalase and peroxidase models. <i>Computational and Theoretical Chemistry</i> , 2003, 632, 323-333. | 1.5 | 4 |
| 1459 | Spectroscopic constants and molecular properties of AlC and SiC in their ground state. <i>Computational and Theoretical Chemistry</i> , 2003, 633, 67-71. | 1.5 | 11 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1460 | VCD technique in determining intermolecular H-bond geometry: a DFT study. Computational and Theoretical Chemistry, 2003, 637, 81-89. | 1.5 | 20 |
| 1461 | Chiral allenes: theoretical VCD and IR spectra. Computational and Theoretical Chemistry, 2003, 635, 151-159. | 1.5 | 13 |
| 1462 | Energy density analysis (EDA) of proton transfer reactions in malonaldehyde, tropolone, and 9-hydroxyphenalenone. Computational and Theoretical Chemistry, 2003, 637, 27-35. | 1.5 | 22 |
| 1463 | A computational investigation on the Lewis acidity of fluoro- and chloronitrenium ions. Computational and Theoretical Chemistry, 2003, 635, 221-227. | 1.5 | 5 |
| 1464 | A theoretical study of gas-phase basicities and proton affinities of alkali metal oxides and hydroxides. Computational and Theoretical Chemistry, 2003, 638, 119-128. | 1.5 | 11 |
| 1465 | Determination of the most stable structures of selected hydroxypyrones and their cations and anions. Computational and Theoretical Chemistry, 2003, 639, 87-100. | 1.5 | 31 |
| 1466 | Computational study of the structural and vibrational properties of ten and twelve vertex closo-carboranes. Chemical Physics, 2003, 286, 45-61. | 0.9 | 26 |
| 1467 | Density functional study of the vibrational frequencies of $\hat{I}\pm$ -Keggin heteropolyanions. Chemical Physics, 2003, 287, 55-69. | 0.9 | 111 |
| 1468 | X-ray, MP2 and DFT studies of the structure and vibrational spectra of trigonellinium chloride. Chemical Physics, 2003, 289, 201-219. | 0.9 | 21 |
| 1469 | 3d-Metal monocarbonyls MCO, MCO ⁺ , and MCO ²⁺ (M=Sc to Cu): comparative bond strengths and catalytic ability to produce CO ₂ in reactions with CO. Chemical Physics, 2003, 290, 47-58. | 0.9 | 26 |
| 1470 | Interaction of carbon atoms with Fe ⁿ , Fe ⁿ⁺ , and Fe ⁿ⁺ clusters (n=1-6). Chemical Physics, 2003, 291, 27-40. | 0.9 | 49 |
| 1471 | A TDDFT study of the lowest excitation energies of polycyclic aromatic hydrocarbons. Chemical Physics, 2003, 292, 11-21. | 0.9 | 283 |
| 1472 | Density functional and ab initio study of the tautomeric forms of 3-acetyl tetronic and 3-acetyl tetramic acids. Chemical Physics, 2003, 293, 355-363. | 0.9 | 16 |
| 1473 | Theoretical study of phototoxic reactions of psoralens. Journal of Photochemistry and Photobiology A: Chemistry, 2003, 154, 235-243. | 2.0 | 105 |
| 1474 | On the contribution of intramolecular H-bonding entropy to the conformational stability of alanine conformations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 1387-1397. | 2.0 | 38 |
| 1475 | A coupled-cluster study of the structure and vibrational spectra of pyrazole and imidazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 2009-2025. | 2.0 | 19 |
| 1476 | Active copper species in 1-butene skeletal isomerization: comparison between copper-modified MCM-41 and beta catalysts. Microporous and Mesoporous Materials, 2003, 60, 159-171. | 2.2 | 35 |
| 1477 | Electron-impact total ionization cross-sections of the chlorofluoromethanes. International Journal of Mass Spectrometry, 2003, 222, 189-200. | 0.7 | 31 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1478 | Metastable states of dimethyloxonium, (CH ₃) ₂ OH. International Journal of Mass Spectrometry, 2003, 222, 49-61. | 0.7 | 20 |
| 1479 | Theoretical interpretation of the observed diastereoisomeric differentiation of cis- and trans-2-methylcyclohexanol in the gas phase mediated by scandium(I). International Journal of Mass Spectrometry, 2003, 222, 383-396. | 0.7 | 4 |
| 1480 | Gas-phase kinetic measurements and quantum chemical calculations of the ligation of Ni ⁺ , Cu ⁺ , Ni ⁺ (pyrrole) _{1,2} and Cu ⁺ (pyrrole) _{1,2} with O ₂ and CO. International Journal of Mass Spectrometry, 2003, 227, 161-173. | 0.7 | 10 |
| 1481 | Binding energies of Cu ⁺ to saturated and $\hat{1}\pm, \hat{1}^2$ -unsaturated alkanes, silanes and germanes. International Journal of Mass Spectrometry, 2003, 227, 401-412. | 0.7 | 26 |
| 1482 | Condensation reaction vs. ligand exchange with first-row transition metal cations: a theoretical study of Cu ⁺ heteroleptic model complexes. International Journal of Mass Spectrometry, 2003, 227, 587-600. | 0.7 | 3 |
| 1483 | Beryllium-helium cations: computational evidence for a large class of thermodynamically stable species. International Journal of Mass Spectrometry, 2003, 228, 415-427. | 0.7 | 19 |
| 1484 | Structure, thermochemistry, and reactivity of MSn ⁺ cations (M=V, Mo; n=1-3) in the gas phase. International Journal of Mass Spectrometry, 2003, 228, 439-456. | 0.7 | 30 |
| 1485 | Generation of neutrals from anionic precursors in the gas phase. International Journal of Mass Spectrometry, 2003, 228, 467-485. | 0.7 | 9 |
| 1486 | Bonding interactions in Ag ⁺ (O ₂) _n and Ag ²⁺ (O ₂) _n clusters: experiment and theory. International Journal of Mass Spectrometry, 2003, 228, 865-877. | 0.7 | 23 |
| 1487 | Density Functional Theory investigation of guanosine triphosphate models Catalytic role of Mg ²⁺ ions in phosphate ester hydrolysis. Journal of Molecular Catalysis A, 2003, 204-205, 409-417. | 4.8 | 8 |
| 1488 | Tailoring transition metal complexes for non linear optics applications A theoretical investigation of the electronic structure of M(CO) _x ClyL complexes (M = Cr, W, Re, Ru, Os, Rh, Ir; L = Pyz, PyzBF ₃ , BPE,) Tj ETQq0 0.8 BT / Overlock 10 T | 0.8 | 10 |
| 1489 | Alkane- and areneoxodiazonium ions: experimental results leading to anab initio theoretical investigation. Journal of Physical Organic Chemistry, 2003, 16, 491-497. | 0.9 | 5 |
| 1490 | An experimental and theoretical study of the preferred hydrogen bonding site of methyl isothiocyanate. Journal of Physical Organic Chemistry, 2003, 16, 608-614. | 0.9 | 6 |
| 1491 | Structure and stability of [C ₂ H ₄ N] ⁺ singlet-state cations: Comparison between DFT and high-level ab initio calculations. International Journal of Quantum Chemistry, 2003, 91, 438-445. | 1.0 | 3 |
| 1492 | DFT study of electronic spectra and excited-state properties of some 1,8-naphthalimide derivatives. International Journal of Quantum Chemistry, 2003, 91, 446-450. | 1.0 | 11 |
| 1493 | Heterolytic activation of C-H bond in methane with (HN?CHCH?NH)M(CH ₃) (M = Pd ⁺ , Pt ⁺ , Rh ⁺ , Ir ⁺ , Rh,) Tj ETQq1 1 0.784314 rgBT / Overlock 10 T Chemistry, 2003, 92, 391-399. | 1.0 | 15 |
| 1494 | Density Functional Theory Calculations of the Barrier to Atropisomerism of a Dibenzo[d, f][1, 3, 2]dioxaphosphepin Moiety: a Tool for Rational Ligand Design. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2003, 629, 2535-2538. | 0.6 | 8 |
| 1495 | Title is missing!. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2003, 629, 803-815. | 0.6 | 8 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1496 | Direct dynamics study of hydrogen abstraction using density functional theory: reaction. <i>Chemical Physics</i> , 2003, 286, 173-180. | 0.9 | 7 |
| 1497 | Probing hydrogen bonding to quinone anion radicals by ¹ H and ² H ENDOR spectroscopy at 35 GHz. <i>Chemical Physics</i> , 2003, 294, 401-413. | 0.9 | 64 |
| 1498 | Relative Reactivity of Peracids versus Dioxiranes (DMDO and TFDO) in the Epoxidation of Alkenes. A Combined Experimental and Theoretical Analysis. <i>Journal of the American Chemical Society</i> , 2003, 125, 924-934. | 6.6 | 63 |
| 1499 | The role of submicrometer aerosols and macromolecules in H ₂ formation in the titan haze. <i>Icarus</i> , 2003, 161, 468-468. | 1.1 | 0 |
| 1500 | NMR Shieldings and Electron Correlation Reveal Remarkable Behavior on the Part of the Flavin N5 Reactive Center. <i>Journal of Physical Chemistry B</i> , 2003, 107, 854-863. | 1.2 | 15 |
| 1501 | Predicting aqueous solubilities from aqueous free energies of solvation and experimental or calculated vapor pressures of pure substances. <i>Journal of Chemical Physics</i> , 2003, 119, 1661-1670. | 1.2 | 97 |
| 1502 | Full configuration interaction potential energy curves for breaking bonds to hydrogen: An assessment of single-reference correlation methods. <i>Journal of Chemical Physics</i> , 2003, 118, 1610-1619. | 1.2 | 115 |
| 1503 | Decarboxylation of carbonyloxy radicals: a density functional study. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 3891-3896. | 1.3 | 10 |
| 1504 | Fluorescence kinetics of aqueous solutions of tetracycline and its complexes with Mg ²⁺ and Ca ²⁺ -This paper is dedicated to Professor Fred Lewis on the event of his 60th birthday.. <i>Photochemical and Photobiological Sciences</i> , 2003, 2, 1107. | 1.6 | 61 |
| 1505 | Robust and Affordable Multicoefficient Methods for Thermochemistry and Thermochemical Kinetics: The MCCM/3 Suite and SAC/3. <i>Journal of Physical Chemistry A</i> , 2003, 107, 3898-3906. | 1.1 | 252 |
| 1506 | N-C Bond Dissociation Energies and Kinetics in Amide and Peptide Radicals. Is the Dissociation a Non-ergodic Process?. <i>Journal of the American Chemical Society</i> , 2003, 125, 5954-5963. | 6.6 | 201 |
| 1507 | Structure, Deprotonation Energy, and Cation Affinity of an Ethynyl-Expanded Cubane. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4957-4961. | 1.1 | 24 |
| 1508 | Fundamental vibrational frequencies of small polyatomic molecules from density-functional calculations and vibrational perturbation theory. <i>Journal of Chemical Physics</i> , 2003, 118, 7215. | 1.2 | 259 |
| 1509 | A Theoretical Study of C ₄ B Isomers. The Interconversion of CCBC and CCCB via Cyclic C ₄ B. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10149-10153. | 1.1 | 23 |
| 1510 | Origin of the Acidity Enhancement of Formic Acid over Methanol: Resonance versus Inductive Effects. <i>Journal of the American Chemical Society</i> , 2003, 125, 2797-2803. | 6.6 | 23 |
| 1511 | Quantum Chemical Characterization of Methane Metathesis in L ₂ MCH ₃ (L = H, Cl, Cp, Cp*; M = Sc, Y, Lu). <i>Organometallics</i> , 2003, 22, 1682-1689. | 1.1 | 47 |
| 1512 | Theoretical Calculation of Accurate Absolute and Relative Gas- and Liquid-Phase O-H Bond Dissociation Enthalpies of 2-Mono- and 2,6-Disubstituted Phenols, Using DFT/B3LYP. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8594-8606. | 1.1 | 74 |
| 1513 | Catalytic Gas Phase Oxidation of Methanol to Formaldehyde. <i>Journal of the American Chemical Society</i> , 2003, 125, 3384-3396. | 6.6 | 228 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1514 | Comparison of the reactivity of O ₂ with a (10,0) and a (9,0) carbon nanotube. <i>Physical Review B</i> , 2003, 68, . | 1.1 | 42 |
| 1515 | A Cornucopia of Cycloadducts: Theoretical Predictions of the Mechanisms and Products of the Reactions of Cyclopentadiene with Cycloheptatriene. <i>Journal of the American Chemical Society</i> , 2003, 125, 8330-8339. | 6.6 | 46 |
| 1516 | Hydrogen Atom Addition to Cytosine, 1-Methylcytosine, and Cytosine-Water Complexes. A Computational Study of a Mechanistic Dichotomy. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9221-9231. | 1.1 | 47 |
| 1517 | Electronic Spectrum of Cobalt-Free Corrins Calculated by TDDFT Method. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1339-1347. | 1.1 | 21 |
| 1518 | Electronic Properties of 4,4'-,5,5'-Tetramethyl-2,2'-biphosphinine (tmbp) in the Redox Series fac-[Mn(Br)(CO) ₃ (tmbp)], [Mn(CO) ₃ (tmbp)] ₂ , and [Mn(CO) ₃ (tmbp)]- Crystallographic, Spectroelectrochemical, and DFT Computational Study. <i>Inorganic Chemistry</i> , 2003, 42, 4442-4455. | 1.9 | 56 |
| 1519 | First Principles Calculations of the Absorption Spectrum of Si ₂₉ H ₃₆ . <i>Nano Letters</i> , 2003, 3, 847-849. | 4.5 | 23 |
| 1520 | Effect of a Charge-Transfer Interaction on the Catalytic Activity of Acyl-CoA Dehydrogenase: A Theoretical Study of the Role of Oxidized Flavin. <i>Journal of Physical Chemistry B</i> , 2003, 107, 13229-13236. | 1.2 | 19 |
| 1521 | Electronic Control of the Regiochemistry in the Heck Reaction. <i>Journal of the American Chemical Society</i> , 2003, 125, 3503-3508. | 6.6 | 83 |
| 1522 | Modeling the Reaction Mechanisms of the Amide Hydrolysis in an N-(o-Carboxybenzoyl)-l-amino Acid. <i>Journal of the American Chemical Society</i> , 2003, 125, 6994-7000. | 6.6 | 37 |
| 1523 | Thermochemistry of Arylselanyl Radicals and the Pertinent Ions in Acetonitrile. <i>Journal of the American Chemical Society</i> , 2003, 125, 2148-2157. | 6.6 | 27 |
| 1524 | Characterization of Hydrogen Bonds in the Interactions between the Hydroperoxyl Radical and Organic Acids. <i>Journal of the American Chemical Society</i> , 2003, 125, 15614-15622. | 6.6 | 32 |
| 1525 | A Wavefunction-Based Criterion for the Detection of Intermolecular Interactions in Molecular Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4141-4146. | 1.1 | 21 |
| 1526 | Experimental and Theoretical Electron Density Distribution and Magnetic Properties of the Butterfly-like Complex [Fe ₄ O ₂ (O ₂ CCMe ₃) ₈ (NC ₅ H ₄ Me) ₂]-2CH ₃ CN. <i>Inorganic Chemistry</i> , 2003, 42, 7593-7601. | 1.9 | 37 |
| 1527 | Assessment of the suitability of using the composite G2, G3, and CBS-RAD methods for predicting activation energies. <i>Chemical Engineering Communications</i> , 2003, 190, 1233-1248. | 1.5 | 5 |
| 1528 | Ortho-CH Activation of Aromatic Ketones, Partially Fluorinated Aromatic Ketones, and Aromatic Imines by a Trihydride-Stanny-Osmium(IV) Complex. <i>Organometallics</i> , 2003, 22, 3753-3765. | 1.1 | 52 |
| 1529 | Electronic Requirements for Oxygen Atom Transfer from Alkyl Hydroperoxides. Model Studies on Multisubstrate Flavin-Containing Monooxygenases. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12851-12861. | 1.2 | 35 |
| 1530 | Agostic vs π -Interactions in Complexes of Ethynylsilanes and Ethynylgermanes with Cu ⁺ in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1370-1376. | 1.1 | 37 |
| 1531 | Self-Association of Isoguanine Nucleobases and Molecular Recognition of Alkaline Ions: A Tetrad vs Pentad Structures. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1025-1031. | 1.1 | 31 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1532 | Fe ⁺ -Mediated Interconversion of n- and i-C ₃ H ₇ OH Preceding Their Gas-Phase Dehydrations: An Experimental and Computational Evidence for Memory Effects and Inherent Asymmetry of Constitutionally Equivalent Methyl Groups. <i>Organometallics</i> , 2003, 22, 693-707. | 1.1 | 35 |
| 1533 | Dehydrogenation of Methane by Gas-Phase Os ⁺ : A Density Functional Study. <i>Organometallics</i> , 2003, 22, 3820-3830. | 1.1 | 57 |
| 1534 | Infrared Spectra of Aluminum Hydrides in Solid Hydrogen: Al ₂ H ₄ and Al ₂ H ₆ . <i>Journal of the American Chemical Society</i> , 2003, 125, 9218-9228. | 6.6 | 117 |
| 1535 | Metal Insertion Route of the Ni + CO ₂ → NiO + CO Reaction. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6708-6713. | 1.1 | 29 |
| 1536 | ER-BOC Calculations of Crystal Bulk Properties from Smallest-Cluster Models. <i>Journal of the American Chemical Society</i> , 2003, 125, 4388-4390. | 6.6 | 9 |
| 1537 | Activation of CH ₄ by Gas-Phase Zr ⁺ and the Thermochemistry of Zr ⁺ Ligand Complexes. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4396-4406. | 1.1 | 42 |
| 1538 | Infrared Spectra of Gallium Hydrides in Solid Hydrogen: GaH _{1,2,3} , Ga ₂ H _{2,4,6} , and the GaH _{2,4} -Anions. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11371-11379. | 1.1 | 57 |
| 1539 | Rates of Catalyzed Processes in Enzymes and Other Cooperative Media. <i>Journal of Physical Chemistry B</i> , 2003, 107, 4437-4443. | 1.2 | 8 |
| 1540 | Preparation and Characterization of Osmium ⁺ Stannyl Polyhydrides: d ₄ Oxidative Addition of Neutral Molecules in a Late Transition Metal. <i>Organometallics</i> , 2003, 22, 2087-2096. | 1.1 | 46 |
| 1541 | Twofold Hydrogen Bridges as Observed in Amide-Templated Rotaxanes. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9634-9640. | 1.1 | 20 |
| 1542 | Similarity and Chirality: A Quantum Chemical Study of Dissimilarity of Enantiomers. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11120-11127. | 1.1 | 42 |
| 1543 | On the Dissolution Processes of Na ₂ I ⁺ and Na ₃ I ⁺ with the Association of Water Molecules: Mechanistic and Energetic Details. <i>Journal of the American Chemical Society</i> , 2003, 125, 3341-3352. | 6.6 | 27 |
| 1544 | Enantioselective [6π]-Photocyclization Reaction of an Acrylanilide Mediated by a Chiral Host. Interplay between Enantioselective Ring Closure and Enantioselective Protonation. <i>Journal of Organic Chemistry</i> , 2003, 68, 1107-1116. | 1.7 | 77 |
| 1545 | Effect of Cations in Infrared and Computational Analysis of Vanadium-Containing Six-Coordinate Oxotungstates. <i>Journal of Physical Chemistry B</i> , 2003, 107, 7747-7752. | 1.2 | 17 |
| 1546 | DFT Computational Study of the Mechanism of Allyl Halides Carbonylation Catalyzed by Nickel Tetracarbonyl. <i>Journal of the American Chemical Society</i> , 2003, 125, 10412-10419. | 6.6 | 26 |
| 1547 | Proton-Coupled Electron Transfer in a Model for Tyrosine Oxidation in Photosystem II. <i>Journal of the American Chemical Society</i> , 2003, 125, 10429-10436. | 6.6 | 100 |
| 1548 | Acrylate Formation via Metal-Assisted C-C Coupling between CO ₂ and C ₂ H ₄ : Reaction Mechanism as Revealed from Density Functional Calculations. <i>Journal of the American Chemical Society</i> , 2003, 125, 14847-14858. | 6.6 | 66 |
| 1549 | Synthesis, Characterization, and Reactivity of (Fluoroalkyl)- and (Fluorocycloalkyl)cobaloximes: Molecular Structure of a (2-Fluorocyclohexyl)cobaloxime Complex and Hindered Rotation of 2-Fluorocycloalkyl Ligands. <i>Organometallics</i> , 2003, 22, 4873-4884. | 1.1 | 14 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1550 | Kinetics Study and Theoretical Modeling of the Diels-Alder Reactions of Cyclopentadiene and Cyclohexadiene with Methyl Vinyl Ketone. The Effects of a Novel Organotungsten Catalyst. <i>Journal of Organic Chemistry</i> , 2003, 68, 3068-3077. | 1.7 | 13 |
| 1551 | Multireference Correlation Calculations for the Ground States of VO ^{+/0/-} Using Correlation Consistent Basis Sets. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5566-5572. | 1.1 | 49 |
| 1552 | Theoretical Study of Nucleophilic Substitution at the Disulfide Bridge of Cyclo-l-cystine. <i>Journal of Organic Chemistry</i> , 2003, 68, 4743-4747. | 1.7 | 30 |
| 1553 | Building Blocks of Eumelanin: Relative Stability and Excitation Energies of Tautomers of 5,6-Dihydroxyindole and 5,6-Indolequinone. <i>Journal of Physical Chemistry B</i> , 2003, 107, 7162-7171. | 1.2 | 75 |
| 1554 | Versatile and Cooperative Reactivity of a Triruthenium Polyhydride Cluster. A Computational Study. <i>Journal of the American Chemical Society</i> , 2003, 125, 9910-9911. | 6.6 | 25 |
| 1555 | Density Functional Study on the Effect of the trans Axial Ligand of B ₁₂ Cofactors on the Heterolytic Cleavage of the Co-C Bond. <i>Journal of Physical Chemistry B</i> , 2003, 107, 306-315. | 1.2 | 48 |
| 1556 | First X-ray Characterization and Theoretical Study of η^5 -Alkyne, Alkynyl-Hydride, and Vinylidene Isomers for the Same Transition Metal Fragment [Cp*Ru(PEt ₃) ₂] ⁺ . <i>Journal of the American Chemical Society</i> , 2003, 125, 3311-3321. | 6.6 | 90 |
| 1557 | Transition Metal Mediated Epoxidation as Test Case for the Performance of Different Density Functionals: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5466-5471. | 1.1 | 51 |
| 1558 | Gas Phase Generation of HCCCS and CCCHS Radicals from Anionic Precursors. The Rearrangement of CCCHS to HCCCS. A Joint Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1879-1886. | 1.1 | 7 |
| 1559 | Theoretical Study of Chlorine Nitrates: Implications for Stratospheric Chlorine Chemistry. <i>Journal of the American Chemical Society</i> , 2003, 125, 10446-10458. | 6.6 | 4 |
| 1560 | Photochemistry of 1-(N,N-Diethylamino)diazene-1,2-diolate: An Experimental and Computational Investigation. <i>Journal of the American Chemical Society</i> , 2003, 125, 14934-14940. | 6.6 | 16 |
| 1561 | Fundamental Reaction Mechanism for Cocaine Hydrolysis in Human Butyrylcholinesterase. <i>Journal of the American Chemical Society</i> , 2003, 125, 2462-2474. | 6.6 | 131 |
| 1562 | Rearrangements of 2-Nitrobenzyl Compounds. 2. Substituent Effects on the Reactions of the Quinonoid Intermediates. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10159-10170. | 1.1 | 18 |
| 1563 | Vibrational Assignments for High Molecular Weight Linear Polyethylenimine (LPEI) Based on Monomeric and Tetrameric Model Compounds. <i>Macromolecules</i> , 2003, 36, 7348-7351. | 2.2 | 40 |
| 1564 | Hybrid Density Functional Theory Predictions of Low-Temperature Dimethyl Ether Combustion Pathways. II. Chain-Branching Energetics and Possible Role of the Criegee Intermediate. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9463-9478. | 1.1 | 64 |
| 1565 | Gas-Phase Chemistry of NH ₂ Cly ⁺ Ions. 3. Structure, Stability, and Reactivity of Protonated Trichloramine. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2085-2092. | 1.1 | 8 |
| 1566 | Spectroscopic and Theoretical Study of Push-Pull Chromophores Containing Thiophene-Based Quinonoid Structures as Electron Spacers. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12175-12183. | 1.2 | 40 |
| 1567 | Orbital Interactions between a C ₆₀ Molecule and Cu(111) Surface. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12672-12679. | 1.2 | 10 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1568 | NH Stretching Vibrations of Jet-Cooled Aniline and Its Derivatives in the Neutral and Cationic Ground States. <i>Journal of Physical Chemistry A</i> , 2003, 107, 3678-3686. | 1.1 | 48 |
| 1569 | Ab Initio Study of an H ₂₄ O ₁₂ Zwitterion. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1348-1358. | 1.1 | 17 |
| 1570 | Computational Insights into the Chemical Structures and Mechanisms of the Chromogenic and Neurotoxic Effects of Aromatic β^3 -diketones. <i>Journal of Physical Chemistry B</i> , 2003, 107, 2853-2861. | 1.2 | 21 |
| 1571 | Electron Affinities, Ionization Energies, and Fragmentation Energies of Fen Clusters ($n = 2 \sim 6$): A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 7013-7023. | 1.1 | 167 |
| 1572 | Adsorption of the Butene Isomers in Faujasite: A Combined ab-Initio Theoretical and Experimental Study. <i>Journal of Physical Chemistry B</i> , 2003, 107, 11065-11071. | 1.2 | 41 |
| 1573 | Modeling Anhydrous and Aqua Copper(II) Amino Acid Complexes: A New Molecular Mechanics Force Field Parametrization Based on Quantum Chemical Studies and Experimental Crystal Data. <i>Inorganic Chemistry</i> , 2003, 42, 2268-2279. | 1.9 | 69 |
| 1574 | Chemical and Photochemical Electron Transfer of New Helianthrone Derivatives: Aspects of Their Photodynamic Activity. <i>Journal of the American Chemical Society</i> , 2003, 125, 1376-1384. | 6.6 | 38 |
| 1575 | Computational Studies of the Chemistry of Syn Acetaldehyde Oxide. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11525-11532. | 1.1 | 37 |
| 1576 | Experimental and Theoretical Characterization of the 3,5-Didehydrobenzoate Anion: A Negatively Charged meta-Benzene. <i>Journal of the American Chemical Society</i> , 2003, 125, 131-140. | 6.6 | 16 |
| 1577 | Replacement of 2,2'-Bipyridine by 1,4-Diazabutadiene Acceptor Ligands: Why the Bathochromic Shift for [(N ⁺ SN)IrCl(C ₅ Me ₅)] ⁺ Complexes but the Hypsochromic Shift for (N ⁺ SN)Ir(C ₅ Me ₅)?. <i>Inorganic Chemistry</i> , 2003, 42, 5185-5191. | 1.9 | 16 |
| 1578 | 5-Cyanoimino-4-oxomethylene-4,5-dihydroimidazole and Nitrosative Guanine Deamination. A Theoretical Study of Geometries, Electronic Structures, and N-Protonation. <i>Journal of Organic Chemistry</i> , 2003, 68, 9882-9892. | 1.7 | 20 |
| 1579 | Mechanism of 1,3-Migration in Allylperoxy Radicals: Computational Evidence for the Formation of a Loosely Bound Radical-Dioxygen Complex. <i>Journal of the American Chemical Society</i> , 2003, 125, 10641-10650. | 6.6 | 20 |
| 1580 | Cycloaddition Reactions of 1-Pyrazoline on the Si(100) 2 \times 1 Surface: A Possible Route to an SiN Interfacial Double Bond. <i>Journal of Physical Chemistry B</i> , 2003, 107, 6853-6858. | 1.2 | 3 |
| 1581 | Stable Compounds of the Lightest Noble Gases: A Computational Investigation of RNBeNg (Ng = He, Ne, Ar, Kr, Xe, Rn). <i>Journal of Physical Chemistry A</i> , 2003, 107, 7843-7857. | 1.1 | 57 |
| 1582 | First principles studies of the surface of galena PbS. <i>Geochimica Et Cosmochimica Acta</i> , 2003, 67, 799-805. | 1.6 | 22 |
| 1583 | Biscyanine dye with Schiff base as new chiroptical materials. <i>Materials Letters</i> , 2003, 57, 1489-1495. | 1.3 | 7 |
| 1584 | Small Representative Benchmarks for Thermochemical Calculations. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8996-8999. | 1.1 | 288 |
| 1585 | Quantum Chemistry Study of Fullerene and Carbon Nanotube Fluorination. <i>Journal of Physical Chemistry B</i> , 2003, 107, 10378-10388. | 1.2 | 54 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1586 | Poly[n]prismanes: A Family of Stable Cage Structures with Half-Planar Carbon Centers. <i>Journal of Organic Chemistry</i> , 2003, 68, 8588-8594. | 1.7 | 64 |
| 1587 | Modeling the Reaction Mechanisms of the Imide Formation in an N-(o-Carboxybenzoyl)-l-amino Acid. <i>Journal of the American Chemical Society</i> , 2003, 125, 3642-3648. | 6.6 | 17 |
| 1588 | Influence of Media and Homoconjugate Pairing on Transition Metal Hydride Protonation. An IR and DFT Study on Proton Transfer to CpRuH(CO)(PCy ₃). <i>Journal of the American Chemical Society</i> , 2003, 125, 7715-7725. | 6.6 | 74 |
| 1589 | Density functional calculations, using Slater basis sets, with exact exchange. <i>Journal of Chemical Physics</i> , 2003, 119, 6475-6481. | 1.2 | 93 |
| 1590 | (Z)-1-Aryl-1-haloalkenes as Intermediates in the Vilsmeier Haloformylation of Aryl Ketones. <i>Organic Letters</i> , 2003, 5, 3387-3390. | 2.4 | 27 |
| 1591 | Nitro-Functionalized Oligothiophenes as a Novel Type of Electroactive Molecular Material: A Spectroscopic, Electrochemical, and Computational Study. <i>Journal of the American Chemical Society</i> , 2003, 125, 2524-2534. | 6.6 | 106 |
| 1592 | A density-functional-theory study of bacteriochlorophyll b. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 4265. | 1.3 | 40 |
| 1593 | Formation of Cyanate (OCN) and Fulminate (ONC) Radicals from Anionic Precursors in the Gas Phase. A Joint Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 76-82. | 1.1 | 16 |
| 1594 | The Spin-Spin Coupling Constants in Ethane, Methanol and Methylamine: A Comparison of DFT, MCSCF and CCSD Results. <i>International Journal of Molecular Sciences</i> , 2003, 4, 143-157. | 1.8 | 39 |
| 1595 | Density functional studies on lanthanide (III) texaphyrins (Ln-Tex ²⁺ , Ln = La, Gd, Lu): structure, stability and electronic excitation spectrum. <i>Molecular Physics</i> , 2003, 101, 2427-2435. | 0.8 | 26 |
| 1596 | Low-Valent Cobalt Complexes with Three Different π Acceptor Ligands: Experimental and DFT Studies of the Reduced and the Low-Lying Excited States of (R-DAB)Co(NO)(CO), R-DAB = Substituted 1,4-Diaza-1,4-butadiene. <i>Inorganic Chemistry</i> , 2003, 42, 3340-3346. | 1.9 | 25 |
| 1597 | Reaction of Criegee Intermediates with Water Vapor: An Additional Source of OH Radicals in Alkene Ozonolysis?. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6176-6182. | 1.1 | 103 |
| 1598 | The Involvement of Metal-to-CO Charge Transfer and Ligand-Field Excited States in the Spectroscopy and Photochemistry of Mixed-Ligand Metal Carbonyls. A Theoretical and Spectroscopic Study of [W(CO) ₄ (1,2-Ethylenediamine)] and [W(CO) ₄ (N,N'-Bis-alkyl-1,4-diazabutadiene)]. <i>Journal of the American Chemical Society</i> , 2003, 125, 4580-4592. | 6.6 | 77 |
| 1599 | Experimental and Theoretical Studies of Bonding and Oxidative Addition of Germanes and Silanes, EH ₄ -nPhn (E = Si, Ge; n = 0-3), to Mo(CO)(diphosphine) ₂ . The First Structurally Characterized Germane η^f Complex. <i>Organometallics</i> , 2003, 22, 5307-5323. | 1.1 | 68 |
| 1600 | Computational Study of the HCCO + NO Reaction: ab Initio MO/vRRKM Calculations of the Total Rate Constant and Product Branching Ratios. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1066-1076. | 1.1 | 32 |
| 1601 | X-ray Structures, Photophysical Characterization, and Computational Analysis of Geometrically Constrained Copper(I)-Phenanthroline Complexes. <i>Inorganic Chemistry</i> , 2003, 42, 4918-4929. | 1.9 | 28 |
| 1602 | Infrared Spectroscopy of Matrix-Isolated Polycyclic Aromatic Compounds and Their Ions. 6. Polycyclic Aromatic Nitrogen Heterocycles. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1486-1498. | 1.1 | 100 |
| 1603 | G3-RAD and G3X-RAD: Modified Gaussian-3 (G3) and Gaussian-3X (G3X) procedures for radical thermochemistry. <i>Journal of Chemical Physics</i> , 2003, 118, 4849-4860. | 1.2 | 276 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1604 | The electron density in flavones I. Baicalein. <i>New Journal of Chemistry</i> , 2003, 27, 1392-1398. | 1.4 | 20 |
| 1605 | Gas Phase Reactivity of Ni ⁺ with Urea. <i>Mass Spectrometry and Theoretical Studies. Journal of Physical Chemistry A</i> , 2003, 107, 9865-9874. | 1.1 | 18 |
| 1606 | Lignin Biosynthesis and Degradation – a Major Challenge for Computational Chemistry. <i>Lecture Notes in Computer Science</i> , 2003, , 137-165. | 1.0 | 8 |
| 1607 | Theoretical Study of Hydration of Cyanamide and Carbodiimide. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1188-1196. | 1.1 | 62 |
| 1608 | Mechanism and Energetics of Intramolecular Hydrogen Transfer in Amide and Peptide Radicals and Cation-Radicals. <i>Journal of the American Chemical Society</i> , 2003, 125, 3353-3369. | 6.6 | 182 |
| 1609 | The Nature and Absolute Hydration Free Energy of the Solvated Electron in Water. <i>Journal of Physical Chemistry B</i> , 2003, 107, 4403-4417. | 1.2 | 107 |
| 1610 | Effects of Basis Set Choice upon the Atomization Energy of the Second-Row Compounds SO ₂ , CCl ₄ , and ClO ₂ for B3LYP and B3PW91. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6720-6724. | 1.1 | 50 |
| 1611 | On the performance of four-component relativistic density functional theory: Spectroscopic constants and dipole moments of the diatomics HX and XY (X,Y=F, Cl, Br, and I). <i>Journal of Chemical Physics</i> , 2003, 118, 10418-10430. | 1.2 | 43 |
| 1612 | Gas phase generation of the neutrals H ₂ CCCCO, HCCCCDO and CCCHCHO from anionic precursors. Rearrangements of HCCCCDO and CCCHCHO. A joint experimental and theoretical study. <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 3111. | 1.5 | 10 |
| 1613 | Shpol'skii spectroscopy and vibrational analysis of [N]phenylenes. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 4563. | 1.3 | 15 |
| 1614 | Experimental and theoretical charge distribution in (Z)-N-methyl-C-phenylnitron. <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 1034-1040. | 1.5 | 20 |
| 1615 | Computational study on the electrocyclic reactions of [16]annulene Electronic supplementary information (ESI) available: cartesian coordinates of all the equilibrium and transition structures optimized at the B3LYP/6-31G(d) level. See http://www.rsc.org/suppdata/ob/b3/b304654k/ . <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 2748. | 1.5 | 8 |
| 1616 | Generation of neutrals from ionic precursors in the gas phase. The rearrangement of CCCCCHO to HCCCCO. <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 1769-1778. | 1.5 | 7 |
| 1617 | X-ray Charge density analysis of the hydrogen bonding motif in 1-(2-hydroxy-5-nitrophenyl)ethanone Electronic supplementary information (ESI) available: multipole population coefficients and pseudoatom parameterization. See http://www.rsc.org/suppdata/ob/b2/b211683a/ . <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 1191-1198. | 1.5 | 36 |
| 1618 | QM/MM calculations of kinetic isotope effects in the chorismate mutase active site. <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 483-487. | 1.5 | 28 |
| 1619 | Structures and harmonic frequencies of sulfur-containing molecules: Assessment of the 1/4 exchange-correlation functional. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 2938-2941. | 1.3 | 4 |
| 1620 | Bonding in the homologous series CsAu, CsAg, and CsCu studied at the 4-component density functional theory and coupled cluster levels. <i>Journal of Chemical Physics</i> , 2003, 119, 9355-9363. | 1.2 | 30 |
| 1621 | Bonding in the ClOO(2A ⁺) and BrOO(2A ⁺) radical: Nonrelativistic single-reference versus relativistic multi-reference descriptions in density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 2320-2326. | 1.3 | 20 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1622 | Theoretical Investigation of the Reactivity of Copper Atoms with Carbon Disulfide. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2711-2715. | 1.1 | 15 |
| 1623 | Reactions of Laser-Ablated Mo and W Atoms, Cations, and Electrons with CO in Excess Neon: Infrared Spectra and Density Functional Calculations on Neutral and Charged Unsaturated Metal Carbonyls. <i>Journal of Physical Chemistry A</i> , 2003, 107, 990-999. | 1.1 | 13 |
| 1624 | An Assessment of Theoretical Methods for the Calculation of Accurate Structures and SN Bond Dissociation Energies of S-Nitrosothiols (RSNOs). <i>Journal of Physical Chemistry A</i> , 2003, 107, 9946-9952. | 1.1 | 57 |
| 1625 | Interaction of Cyclic Cytosine-, Guanine-, Thymine-, Uracil- and Mixed Guanine-Cytosine Base Tetrads with K^{+} , Na^{+} and Li^{+} Ions: A Density Functional Study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2003, 20, 507-517. | 2.0 | 26 |
| 1626 | Aminoallenylidene complexes of ruthenium(II) from the regioselective addition of secondary amines to butatrienylidene intermediates: a combined experimental and theoretical study of the hindered rotation around the CN-bond. <i>Dalton Transactions</i> , 2003, , 2342-2352. | 1.6 | 27 |
| 1627 | Tris(pentafluorophenyl)borane adducts of substituted imidazoles: conformational features and chemical behavior upon deprotonation. <i>Dalton Transactions</i> , 2003, , 1337-1344. | 1.6 | 34 |
| 1628 | Lithiation/silylation of ethyl 2-alkyl-1-trimethylsilylcycloprop-2-ene-1-carboxylate. Experimental and computational study. <i>New Journal of Chemistry</i> , 2003, 27, 1270. | 1.4 | 10 |
| 1629 | Density Functional Theory and its Application to Nuclear Magnetic Resonance Shielding Constants. <i>Annual Reports on NMR Spectroscopy</i> , 2003, , 117-168. | 0.7 | 11 |
| 1630 | An Ab Initio Molecular Orbital Study of Valence Bond Isomers of Silabenzene and Phosphabenzene. Phosphorus, Sulfur and Silicon and the Related Elements, 2003, 178, 869-880. | 0.8 | 4 |
| 1631 | Distributed dispersion: A new approach. <i>Journal of Chemical Physics</i> , 2003, 119, 4620-4628. | 1.2 | 71 |
| 1632 | Theoretical studies of the first-row transition metal phosphides. <i>Journal of Chemical Physics</i> , 2003, 118, 9224-9232. | 1.2 | 31 |
| 1633 | Ab initio molecular dynamics study on the excitation dynamics of psoralen compounds. <i>Journal of Chemical Physics</i> , 2003, 119, 4223-4228. | 1.2 | 12 |
| 1634 | Calculations of nuclear magnetic shielding in paramagnetic molecules. <i>Journal of Chemical Physics</i> , 2003, 118, 2550. | 1.2 | 71 |
| 1635 | Kohn-Sham density-functional study of the adsorption of acetylene and vinylidene on iron clusters, Fen^{+} ($n=1-4$). <i>Journal of Chemical Physics</i> , 2003, 119, 12279-12290. | 1.2 | 17 |
| 1636 | Thermodynamics of ammonia activation by iron cluster cations: Guided ion beam studies of the reactions of Fen^{+} ($n=2-10,14$) with ND_3 . <i>Journal of Chemical Physics</i> , 2003, 119, 8979-8995. | 1.2 | 28 |
| 1637 | Empirical density functional and the adsorption of organic molecules on Si(100). <i>Physical Review B</i> , 2003, 67, . | 1.1 | 18 |
| 1638 | Structural and electronic properties of iron monoxide clusters $FenO$ and $FenO^{+}$ ($n=2-6$): A combined photoelectron spectroscopy and density functional theory study. <i>Journal of Chemical Physics</i> , 2003, 119, 11135-11145. | 1.2 | 55 |
| 1639 | Excited state tautomerism of the DNA base guanine: A restricted open-shell Kohn-Sham study. <i>Journal of Chemical Physics</i> , 2003, 118, 5400-5407. | 1.2 | 57 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1640 | An Ab Initio Molecular Orbital Study of Isophosphinines. Phosphorus, Sulfur and Silicon and the Related Elements, 2003, 178, 485-494. | 0.8 | 0 |
| 1641 | Binding at molecule/gold transport interfaces. I. Geometry and bonding. Journal of Chemical Physics, 2003, 119, 11926-11942. | 1.2 | 65 |
| 1642 | Significance of single-electron energies for the description of CO on Pt(111). Physical Review B, 2003, 68, . | 1.1 | 225 |
| 1643 | Structure of neutral and charged FenCO clusters (n=1â€“6) and energetics of the FenCO+COâ†’FenC+CO2 reaction. Journal of Chemical Physics, 2003, 119, 3681-3690. | 1.2 | 43 |
| 1644 | Mechanisms of metalloenzymes studied by quantum chemical methods. Quarterly Reviews of Biophysics, 2003, 36, 91-145. | 2.4 | 171 |
| 1645 | Development of a modified embedded atom method for bcc transition metals. Journal of Physics Condensed Matter, 2003, 15, 8917-8926. | 0.7 | 8 |
| 1646 | Gas-phase reactivity of lactones: structure and stability of their Cu+complexes. Molecular Physics, 2003, 101, 1249-1258. | 0.8 | 7 |
| 1647 | Computational Studies on the Mechanism of Orotidine Monophosphate Decarboxylase. Advances in Physical Organic Chemistry, 2003, 38, 183-218. | 0.5 | 3 |
| 1648 | Is Allylphosphine a Carbon or a Phosphorus Base in the Gas Phase?. European Journal of Mass Spectrometry, 2003, 9, 245-255. | 0.5 | 5 |
| 1649 | Stereochemical Interactions in Ammonium Dications, Hypervalent Diammonium Cation-Radicals and Ammonium Radicals. A B3-MP2 Computational Study. European Journal of Mass Spectrometry, 2003, 9, 267-277. | 0.5 | 5 |
| 1650 | On the Formation of Cyclobutane Pyrimidine Dimers in UV-irradiated DNA: Why are Thymines More Reactive?Â¶. Photochemistry and Photobiology, 2003, 78, 159. | 1.3 | 47 |
| 1651 | A Theoretical Study of Imidazole- and Thiol-Based Zinc Binding Groups Relevant to Inhibition of Metzincins. Journal of Physical Chemistry B, 2004, 108, 13839-13849. | 1.2 | 18 |
| 1652 | Energies of isoelectronic atomic ions from a successful metageneralized gradient approximation and other density functionals. Physical Review A, 2004, 70, . | 1.0 | 33 |
| 1653 | Quantum effect on the internal proton transfer and structural fluctuation in the H[sub 5][sup +] cluster. Journal of Chemical Physics, 2004, 121, 10991. | 1.2 | 24 |
| 1654 | Magnetic-field dependence of 59Conuclear magnetic shielding in Co(III) complexes. Physical Review A, 2004, 69, . | 1.0 | 19 |
| 1655 | Using the local density approximation and the LYP, BLYP and B3LYP functionals within reference-state one-particle density-matrix theory. Molecular Physics, 2004, 102, 627-639. | 0.8 | 52 |
| 1656 | Resonance Raman spectra of uracil based on Kramersâ€™Kronig relations using time-dependent density functional calculations and multireference perturbation theory. Journal of Chemical Physics, 2004, 120, 11564-11577. | 1.2 | 81 |
| 1657 | Gas phase infrared spectroscopy of mono- and divanadium oxide cluster cations. Journal of Chemical Physics, 2004, 120, 6461-6470. | 1.2 | 110 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1658 | Weak ferromagnetism with very large canting in a chiral lattice: Fe(pyrimidine) ₂ Cl ₂ . <i>Physical Review B</i> , 2004, 69, . | 1.1 | 38 |
| 1659 | Electronic ground states of the V ₂ O ₄ ^{+/0} species from multireference correlation and density functional studies. <i>Journal of Chemical Physics</i> , 2004, 120, 4207-4215. | 1.2 | 47 |
| 1660 | Magnetic-field-induced quadrupole coupling in the nuclear magnetic resonance of noble-gas atoms and molecules. <i>Physical Review A</i> , 2004, 70, . | 1.0 | 5 |
| 1661 | Reference-state one-particle density-matrix theory. <i>Physical Review A</i> , 2004, 69, . | 1.0 | 3 |
| 1662 | A theoretical study of small copper oxide clusters: Cu ₂ O _x (x=1-4). <i>Journal of Chemical Physics</i> , 2004, 120, 2746-2751. | 1.2 | 26 |
| 1663 | Energy density analysis of cluster size dependence of surface-molecule interactions: H ₂ , C ₂ H ₂ , C ₂ H ₄ , and CO adsorption onto Si(100)-(2Å ⁻¹) surface. <i>Journal of Chemical Physics</i> , 2004, 121, 4893-4900. | 1.2 | 29 |
| 1664 | Relativistic Density Functional Calculations on Small Molecules. <i>Theoretical and Computational Chemistry</i> , 2004, 14, 598-655. | 0.2 | 11 |
| 1665 | Methods and Implementation of Robust, High-Precision Gaussian Basis DFT Calculations for Periodic Systems: the GTOFF Code. <i>Theoretical and Computational Chemistry</i> , 2004, , 171-228. | 0.2 | 9 |
| 1666 | Simulating Thermochemistry of p-Benzo-quinone Reduction and Binding of Ubiquinone in the Photosynthetic Reaction Center. <i>ACS Symposium Series</i> , 2004, , 51-69. | 0.5 | 0 |
| 1667 | Calculation of trans-Hydrogen-Bond ¹³ C- ¹⁵ N Three-Bond and Other Scalar ρ -Couplings in Cooperative Peptide Models. A Density Functional Theory Study. <i>Journal of the American Chemical Society</i> , 2004, 126, 14190-14197. | 6.6 | 47 |
| 1668 | Asymmetric Catalysis Special Feature Part I: OH-Pd(0) interaction as a stabilizing factor in palladium-catalyzed allylic alkylations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 5400-5404. | 3.3 | 22 |
| 1669 | Hydration of protonated primary amines: effects of intermolecular and intramolecular hydrogen bonds. <i>International Journal of Mass Spectrometry</i> , 2004, 236, 81-90. | 0.7 | 47 |
| 1670 | Oxidation pathways of adenine and guanine in aqueous solution from first principles electrochemistry. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 4707. | 1.3 | 51 |
| 1671 | Synthesis of (azidomethyl)phenylboronic acids. <i>Russian Chemical Bulletin</i> , 2004, 53, 370-375. | 0.4 | 7 |
| 1672 | Application of the DFT Theory to Study Cobalamin Complexes. <i>Structural Chemistry</i> , 2004, 15, 431-435. | 1.0 | 17 |
| 1673 | Active Sites for the Vapor Phase Beckmann Rearrangement over Mordenite: An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11388-11397. | 1.1 | 46 |
| 1674 | A Sequential Molecular Mechanics/Quantum Mechanics Study of the Electronic Spectra of Amides. <i>Journal of the American Chemical Society</i> , 2004, 126, 13502-13511. | 6.6 | 68 |
| 1675 | A theoretical study of the cis-dihydroxylation mechanism in naphthalene 1,2-dioxygenase. <i>Journal of Biological Inorganic Chemistry</i> , 2004, 9, 439-452. | 1.1 | 104 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1676 | A theoretical study of spin states in Ni-S4 complexes and models of the [NiFe] hydrogenase active site. <i>Journal of Biological Inorganic Chemistry</i> , 2004, 9, 873-884. | 1.1 | 52 |
| 1677 | Isomeric differentiation and quantification of $\hat{1}\pm$, $\hat{1}^2$ -amino acid-containing tripeptides by the kinetic method: alkali metal-bound dimeric cluster ions. <i>International Journal of Mass Spectrometry</i> , 2004, 231, 103-111. | 0.7 | 40 |
| 1678 | Metathesis activity of monomeric Mo-methylidene centres on (100) and (110)C surfaces of $\hat{1}^3$ -Al ₂ O ₃ â€“â€“a comparative DFT study. <i>Surface Science</i> , 2004, 562, 101-112. | 0.8 | 16 |
| 1679 | Ring strain energies: substituted rings, norbornanes, norbornenes and norbornadienes. <i>Tetrahedron</i> , 2004, 60, 8103-8112. | 1.0 | 225 |
| 1680 | Interpretation of the temperature-dependent color of blue copper protein mutants. <i>Journal of Inorganic Biochemistry</i> , 2004, 98, 896-902. | 1.5 | 21 |
| 1681 | Spectroscopic constants and molecular properties of diatomic carbides. <i>Journal of Molecular Spectroscopy</i> , 2004, 224, 1-6. | 0.4 | 13 |
| 1682 | Degenerate propene metathesis on Mo-alkylidene centres of molybdenaâ€“alumina catalystâ€“a DFT study. <i>Journal of Molecular Catalysis A</i> , 2004, 218, 91-100. | 4.8 | 16 |
| 1683 | Conformational analysis of methylphenidate: comparison of molecular orbital and molecular mechanics methods. <i>Journal of Computer-Aided Molecular Design</i> , 2004, 18, 719-738. | 1.3 | 12 |
| 1684 | Computational investigation of the vibrational and electronic states of S ₂ N ₂ . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2004, 60, 471-480. | 2.0 | 9 |
| 1685 | Vibrational analysis of the chorismate rearrangement: relaxed force constants, isotope effects and activation entropies calculated for reaction in vacuum, water and the active site of chorismate mutase. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 592-601. | 0.9 | 28 |
| 1686 | 298â€“K enthalpies of formation of monofluorinated alkanes: theoretical predictions for methyl, ethyl, isopropyl and tert-butyl fluoride. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 656-664. | 0.9 | 21 |
| 1687 | Catalytic dehydrogenation of ethane over mononuclear Cr(III) surface sites on silica. part I. Câ€“H activation by $\hat{1}^f$ â€“bond metathesis. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 990-1006. | 0.9 | 44 |
| 1688 | The formation of R ₄ CCCO and CCC(O)R(Râ€“=â€“Me, Ph) neutral radicals from ionic precursors in the gas phase: the rearrangement of CCC(O)Ph. <i>Rapid Communications in Mass Spectrometry</i> , 2004, 18, 1008-1016. | 0.7 | 4 |
| 1689 | Application of accurate MP2 energies for closed-shell atoms in examinations of density functionals for 3d 10 electron ions. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 277-287. | 1.0 | 7 |
| 1690 | Theoretical investigation of the structures and properties of fluoromethyl peroxy radicals. <i>International Journal of Quantum Chemistry</i> , 2004, 98, 502-514. | 1.0 | 4 |
| 1691 | Relative energies, stereoelectronic interactions, and conformational interconversion in silacycloalkanes. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 720-732. | 1.0 | 26 |
| 1692 | Modeling of the molecular structure and catalytic activity of the new fullerene-based catalyst (?2-c60)pd(PPh ₃) ₂ : An application in the reaction of selective hydrogenation of acetylenic alcohols. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 810-817. | 1.0 | 13 |
| 1693 | Determination of the absolute configuration of calliactine by quantum chemical calculations. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 1104-1113. | 1.0 | 11 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1694 | The Binary Group 4 Azides [Ti(N ₃) ₄], [P(C ₆ H ₅) ₄][Ti(N ₃) ₅], and [P(C ₆ H ₅) ₄] ₂ [Ti(N ₃) ₆] and on Linear Tii£zNi£zNN Coordination. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 3148-3152. | 7.2 | 73 |
| 1695 | The [NH ₃ Cl] ⁺ Ion. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 5213-5217. | 7.2 | 9 |
| 1696 | Terminal Heck Vinylations of Chelating Vinyl Ethers. <i>Advanced Synthesis and Catalysis</i> , 2004, 346, 1773-1781. | 2.1 | 24 |
| 1699 | On the Electronic Structure of Mesitylnickel Complexes of π -Diimines Combining Structural Data, Spectroscopy and Calculations. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 2784-2796. | 1.0 | 28 |
| 1700 | EPR Insensitivity of the Metal-Nitrosyl Spin-Bearing Moiety in Complexes [LnRuII-NO \cdot] _k . <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 2902-2907. | 1.0 | 35 |
| 1701 | Roesky's Ketone: Structure, Aromaticity and Reactivity. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 3798-3805. | 1.0 | 15 |
| 1702 | A Comparison of Transition States During H-Atom Abstraction of Monophenols and Catechol by Methyl Radical. <i>European Journal of Organic Chemistry</i> , 2004, 2004, 120-128. | 1.2 | 10 |
| 1703 | Hydrogen Migration Over Organic Tapes: [1,5] Sigmatropic Shiftamers. <i>European Journal of Organic Chemistry</i> , 2004, 2004, 273-280. | 1.2 | 6 |
| 1704 | Diastereoselective Synthesis of Thieno[3 α :2,2 β :4,5]cyclopenta[1,2-d][1,3]oxazolines \hat{r} New Ligands for the Copper-Catalyzed Asymmetric Conjugate Addition of Diethylzinc to Enones. <i>European Journal of Organic Chemistry</i> , 2004, 2004, 4442-4451. | 1.2 | 20 |
| 1705 | On the Bond-Stretch Isomerism in the Benzo[1,2:4,5]dicyclobutadiene System \hat{r} An ab initio MR-AQCC Study. <i>ChemPhysChem</i> , 2004, 5, 975-981. | 1.0 | 18 |
| 1706 | Oxygenolysis of Flavonoid Compounds: DFT Description of the Mechanism for Quercetin. <i>ChemPhysChem</i> , 2004, 5, 1726-1733. | 1.0 | 40 |
| 1707 | FN+Cl Ions from Ionized F ₂ NCl: a Computational Investigation on the Structure and Reactivity toward H ₂ O. <i>Helvetica Chimica Acta</i> , 2004, 87, 1467-1482. | 1.0 | 3 |
| 1708 | Computational Interpretation of Vibrational Optical Activity: The ROA Spectra of (4S)-4-Methylisochromane and the (4S)-Isomers of Galaxolide \hat{A} [®] . <i>Helvetica Chimica Acta</i> , 2004, 87, 2208-2234. | 1.0 | 55 |
| 1709 | Systematic quantum chemical study of DNA-base tautomers. <i>Journal of Computational Chemistry</i> , 2004, 25, 83-99. | 1.5 | 173 |
| 1710 | Theoretical study on the excited states of psoralen compounds bonded to a thymine residue. <i>Journal of Computational Chemistry</i> , 2004, 25, 179-188. | 1.5 | 12 |
| 1711 | Class I ribonucleotide reductase revisited: The effect of removing a proton on Glu441. <i>Journal of Computational Chemistry</i> , 2004, 25, 311-321. | 1.5 | 31 |
| 1712 | Second-order atomic Fukui indices from the electron-pair density in the framework of the atoms in molecules theory. <i>Journal of Computational Chemistry</i> , 2004, 25, 439-446. | 1.5 | 13 |
| 1713 | Performance of the Harris functional for extended basis sets at the Hartree \hat{r} Fock and density functional levels. <i>Journal of Computational Chemistry</i> , 2004, 25, 637-648. | 1.5 | 0 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1714 | Reduced basis set for the gold atom in cluster complexes. <i>Journal of Computational Chemistry</i> , 2004, 25, 899-906. | 1.5 | 6 |
| 1715 | Improvement of parallelization performance of GAMESS: Global sum and (semi-)direct integral calculation in multireference perturbation calculation. <i>Journal of Computational Chemistry</i> , 2004, 25, 1175-1183. | 1.5 | 2 |
| 1716 | Improved model core potentials for the second- and third-row transition metals. <i>Journal of Computational Chemistry</i> , 2004, 25, 1206-1213. | 1.5 | 28 |
| 1717 | Systematic study of vibrational frequencies calculated with the self-consistent charge density functional tight-binding method. <i>Journal of Computational Chemistry</i> , 2004, 25, 1858-1864. | 1.5 | 80 |
| 1718 | Quantum chemical/vRRKM study on the thermal decomposition of cyclopentadiene. <i>International Journal of Chemical Kinetics</i> , 2004, 36, 139-151. | 1.0 | 21 |
| 1719 | Indirect nuclear spin-spin coupling constants in 1,2-diboretane-3-ylidene, a homoaromatic system with σ and π 3c/2e bonds. Comparison of experimental data with calculations using density functional theory(DFT). <i>Magnetic Resonance in Chemistry</i> , 2004, 42, 490-495. | 1.1 | 18 |
| 1720 | Quadricyclane Radical Cation Rearrangements: A Computational Study of the Transformations to 1,3,5-Cycloheptatriene and Norbornadiene. <i>Chemistry - A European Journal</i> , 2004, 10, 681-688. | 1.7 | 4 |
| 1721 | The Diphosphate Monoanion in the Gas Phase: A Joint Mass Spectrometric and Theoretical Study. <i>Chemistry - A European Journal</i> , 2004, 10, 840-850. | 1.7 | 5 |
| 1722 | Metal-Induced Tautomerization of p-quinone Compounds: Experimental Evidence from CuI and ReI Complexes of Azophenine and DFT Studies. <i>Chemistry - A European Journal</i> , 2004, 10, 149-154. | 1.7 | 51 |
| 1723 | DFT Description of the Electronic Structure and Spectromagnetic Properties of Strongly Correlated Electronic Systems: NiII, CuII and ZnII-Dioxolene Complexes. <i>Chemistry - A European Journal</i> , 2004, 10, 1472-1480. | 1.7 | 11 |
| 1724 | Vibrational and Quantum-Chemical Study of Nonlinear Optical Chromophores Containing Dithienothiophene as the Electron Relay. <i>Chemistry - A European Journal</i> , 2004, 10, 3805-3816. | 1.7 | 44 |
| 1725 | Synthesis, Structure, and Dynamics of Six-Membered Metallocoronands and Metallodendrimers of Iron and Indium. <i>Chemistry - A European Journal</i> , 2004, 10, 1899-1905. | 1.7 | 88 |
| 1726 | A Photochemical Activation Scheme of Inert Dinitrogen by Dinuclear RuII and FeII Complexes. <i>Chemistry - A European Journal</i> , 2004, 10, 4443-4453. | 1.7 | 48 |
| 1727 | Binding H ₂ , N ₂ , H ₂ ⁺ , and BH ₃ to Transition-Metal Sulfur Sites: Synthesis and Properties of [Ru(L)(PR ₃) ₂ (N ₂ Me ₂ S ₂) ⁺] Complexes (L=1,2-H ₂ , H ₂ ⁺ , BH ₃ ; R=Cy,iPr). <i>Chemistry - A European Journal</i> , 2004, 10, 4214-4224. | 1.7 | 20 |
| 1728 | Synthesis and Determination of the Absolute Configuration of Fugomycin and Desoxyfugomycin: CD Spectroscopy and Fungicidal Activity of Butenolides. <i>Chemistry - A European Journal</i> , 2004, 10, 4584-4593. | 1.7 | 31 |
| 1729 | Controlling the Conformation of Arylamides: Computational Studies of Intramolecular Hydrogen Bonds between Amides and Ethers or Thioethers. <i>Chemistry - A European Journal</i> , 2004, 10, 5008-5016. | 1.7 | 36 |
| 1730 | Ligand Bite Governs Enantioselectivity: Electronic and Steric Control in Pd-Catalyzed Allylic Alkylations by Modular Fenchyl Phosphinites (FENOPs). <i>Chemistry - A European Journal</i> , 2004, 10, 5422-5431. | 1.7 | 43 |
| 1731 | Theory and Experiment in Concert: Templated Synthesis of Amide Rotaxanes, Catenanes, and Knots. <i>Chemistry - A European Journal</i> , 2004, 10, 4777-4789. | 1.7 | 62 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1732 | From Allylic Alcohols to Aldols by Using Iron Carbonyls as Catalysts: Computational Study on a Novel Tandem Isomerization-Aldolization Reaction. <i>Chemistry - A European Journal</i> , 2004, 10, 5795-5803. | 1.7 | 32 |
| 1733 | Isotope Exchange in Ionised CO ₂ /COMixtures: The Role of Asymmetrical C ₂ O ₃ ⁺ Ions. <i>Chemistry - A European Journal</i> , 2004, 10, 6411-6421. | 1.7 | 6 |
| 1734 | Electronic Structure and Chain-Length Effects in Diplatinum Polyynediyl Complexes <i>trans,trans</i> -[(X)(R ₃ P) ₂ Pt(C≡C) _n Pt(PR ₃) ₂ (X)]: A Computational Investigation. <i>Chemistry - A European Journal</i> , 2004, 10, 6510-6522. | 1.7 | 75 |
| 1735 | Theoretical and experimental study of the conformational, structural analysis and vibrational spectra of 1,2-bis(1,2,4-triazole-1-yl)ethane. <i>Journal of Molecular Structure</i> , 2004, 691, 159-163. | 1.8 | 23 |
| 1736 | The structures of the azido-, isocyanato- and isothiocyanato-derivatives of germane, stannane and plumbane and their trimethyl derivatives: a comparison of ab initio results with experiment, and with the methane and silane analogs. <i>Journal of Molecular Structure</i> , 2004, 692, 43-56. | 1.8 | 10 |
| 1737 | Spectroscopic and structural investigations on [(DD18C6)H ₂]I ₈ formed in the reaction of N,N- ϵ -dibenzylated diazacrown ether (DD18C6) with iodine. <i>Inorganica Chimica Acta</i> , 2004, 357, 4144-4150. | 1.2 | 14 |
| 1738 | Sulfurous acid (H ₂ SO ₃) on Io?. <i>Icarus</i> , 2004, 169, 242-249. | 1.1 | 20 |
| 1739 | Synthesis of a new zwitterionic cyclopentadienyl-imidazolium compound and isolation of the 3,3- ϵ -(<i>trans</i> -3,5-cyclopentenyl)di(1- <i>tert</i> -butylimidazolium)bromide intermediate. <i>Tetrahedron Letters</i> , 2004, 45, 8695-8698. | 0.7 | 8 |
| 1740 | Rutheniumtetraoxide oxidation of alkenes: a density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2004, 671, 197-204. | 1.5 | 16 |
| 1741 | Theoretical studies on structural properties and electron transfer reactivity of the C ₄ H ₄ O/C ₄ H ₄ O ⁺ furan coupling pair. <i>Computational and Theoretical Chemistry</i> , 2004, 671, 161-172. | 1.5 | 2 |
| 1742 | A DFT study of the tautomeric equilibria of substituted pyridone-like derivatives: sulphur versus oxygen and imino effect. <i>Computational and Theoretical Chemistry</i> , 2004, 709, 129-134. | 1.5 | 6 |
| 1743 | Prediction of gas phase thermodynamic function of polychlorinated dibenzo-p-dioxins using DFT. <i>Computational and Theoretical Chemistry</i> , 2004, 672, 97-104. | 1.5 | 51 |
| 1744 | Theoretical elucidation of structure-activity relationship for coumarins to scavenge peroxy radical. <i>Computational and Theoretical Chemistry</i> , 2004, 673, 199-202. | 1.5 | 36 |
| 1745 | Structure, spectra and the effects of twisting of β -sheet peptides. A density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2004, 675, 95-105. | 1.5 | 54 |
| 1746 | Theoretical study on analytical potential function and spectroscopic parameters for CaF molecule. <i>Computational and Theoretical Chemistry</i> , 2004, 678, 183-188. | 1.5 | 28 |
| 1747 | On simple, accurate calculations of atomic charges, bond properties and molecular energies. IV. Butane gauche interactions and vibrational energies of alkylcyclohexanes and related polycyclic hydrocarbons. <i>Computational and Theoretical Chemistry</i> , 2004, 682, 153-158. | 1.5 | 6 |
| 1748 | Silylisocyanates and silylthiocyanates: a comparative theoretical study. <i>Computational and Theoretical Chemistry</i> , 2004, 682, 17-27. | 1.5 | 5 |
| 1749 | First-principles studies of C-13 NMR chemical shift tensors of amino acids in crystal state. <i>Computational and Theoretical Chemistry</i> , 2004, 682, 73-82. | 1.5 | 28 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1750 | On simple, accurate calculations of atomic charges, bond properties and molecular energies. V. Conformational features of alkylcyclohexanes and related polycyclic hydrocarbons. Computational and Theoretical Chemistry, 2004, 685, 175-184. | 1.5 | 2 |
| 1751 | 5-Hydroxycyclooctanone's hemicetal rearrangement: ab initio mechanistic study. Computational and Theoretical Chemistry, 2004, 685, 139-145. | 1.5 | 1 |
| 1752 | Insight into the stability and structural properties of HPS3 isomers from density functional theory computations. Computational and Theoretical Chemistry, 2004, 712, 1-7. | 1.5 | 0 |
| 1753 | Molecular structure and vibrational spectra of 3-chloro-4-methyl aniline by density functional theory and ab initio Hartree-Fock calculations. Computational and Theoretical Chemistry, 2004, 711, 25-32. | 1.5 | 66 |
| 1754 | Reactions of chelated η^3 -pentadienyl iron complexes with nucleophiles. Journal of Organometallic Chemistry, 2004, 689, 575-584. | 0.8 | 7 |
| 1755 | The counterion influence on the CH-activation of methane by palladium(II) biscarbene complexes: structures, reactivity and DFT calculations. Journal of Organometallic Chemistry, 2004, 689, 1418-1424. | 0.8 | 101 |
| 1756 | Structure and UV-Vis spectroscopy of nitrosylthiolatoferrate mononuclear complexes. Journal of Organometallic Chemistry, 2004, 689, 1702-1713. | 0.8 | 19 |
| 1757 | Electronic excitation spectra and singlet-triplet coupling in psoralen and its sulfur and selenium analogs. Journal of Photochemistry and Photobiology A: Chemistry, 2004, 167, 201-212. | 2.0 | 21 |
| 1758 | Meerwein reaction of phosphonium ions with epoxides and thioepoxides in the gas phase. Journal of the American Society for Mass Spectrometry, 2004, 15, 398-405. | 1.2 | 12 |
| 1759 | Modeling deoxyribose radicals by neutralization-reionization mass spectrometry. Part 1. Preparation, dissociations, and energetics of 2-hydroxyoxolan-2-yl radical, neutral isomers, and cations. Journal of the American Society for Mass Spectrometry, 2004, 15, 1055-1067. | 1.2 | 7 |
| 1760 | Modeling deoxyribose radicals by neutralization-reionization mass spectrometry. Part 2. Preparation, dissociations, and energetics of 3-hydroxyoxolan-3-yl radical and cation. Journal of the American Society for Mass Spectrometry, 2004, 15, 1068-1079. | 1.2 | 5 |
| 1761 | Crystal and molecular structure, hydrogen bonding and electrostatic interactions of bis(pyridine) Tj ETQq1 1 0.784314 rgBT /Overlock 18 | 1.8 | 18 |
| 1762 | Crystal and molecular structure, hydrogen bonding and electrostatic interactions of bis(trigonelline) hydrogen perchlorate monohydrate. Journal of Molecular Structure, 2004, 704, 45-52. | 1.8 | 22 |
| 1763 | X-Ray, MP2 and DFT studies of the structure and vibrational spectra of homarinium chloride. Journal of Molecular Structure, 2004, 700, 109-125. | 1.8 | 15 |
| 1764 | Thermochemistry, singlet-triplet gap and crystal structure of (tetramethylethylenediamine)nickelbis(acetylacetonate) [(TMEDA)Ni(acac) ₂]. Inorganic Chemistry Communication, 2004, 7, 296-301. | 1.8 | 16 |
| 1765 | Allenylidene complexes of ruthenium: synthesis, spectroscopy and electron transfer properties. Coordination Chemistry Reviews, 2004, 248, 1565-1583. | 9.5 | 94 |
| 1766 | The NMR indirect nuclear spin-spin coupling constants for some small rigid hydrocarbons: molecular equilibrium values and vibrational corrections. Chemical Physics, 2004, 296, 53-62. | 0.9 | 63 |
| 1767 | Calculation of $\sigma \rightarrow \sigma^*$ excitation energies of organic molecules by CIS(D) quantum chemical methods. Chemical Physics, 2004, 305, 223-230. | 0.9 | 91 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1768 | Possible molecular hydrogen formation mediated by the inner and outer carbon atoms of typical PAH cations. <i>Chemical Physics</i> , 2004, 305, 307-316. | 0.9 | 59 |
| 1769 | Reorganizational dynamics of multilamellar lipid bilayer assemblies using continuously scanning Fourier transform infrared spectroscopic imaging. <i>Chemistry and Physics of Lipids</i> , 2004, 130, 167-174. | 1.5 | 18 |
| 1770 | A computational study on the acceleration of the Prins reaction by indium trichloride. <i>Comptes Rendus Chimie</i> , 2004, 7, 885-893. | 0.2 | 1 |
| 1771 | Density-functional calculations of NMR shielding constants using the localized Hartree-Fock method. <i>Chemical Physics Letters</i> , 2004, 383, 115-121. | 1.2 | 47 |
| 1772 | Predicting energies and geometries for reactions involved in atmosphere chemistry: a comparison study between hybrid DFT methods. <i>Chemical Physics Letters</i> , 2004, 384, 20-24. | 1.2 | 31 |
| 1773 | Structures of the formic acid trimer. <i>Chemical Physics Letters</i> , 2004, 386, 162-168. | 1.2 | 40 |
| 1774 | Hydrogen-bonded complexes of glycolic acid with one and two water molecules. <i>Chemical Physics Letters</i> , 2004, 387, 142-148. | 1.2 | 19 |
| 1775 | Theoretical enthalpies of formation and O-H bond dissociation enthalpy of an Î±-tocopherol model and its free radical. <i>Chemical Physics Letters</i> , 2004, 388, 274-278. | 1.2 | 12 |
| 1776 | Current-voltage curves for molecular junctions: the effect of Cl substituents and basis set composition. <i>Chemical Physics Letters</i> , 2004, 388, 427-429. | 1.2 | 29 |
| 1777 | Calculation of the electronic spectra of molecules in solution and on surfaces. <i>Chemical Physics Letters</i> , 2004, 390, 124-129. | 1.2 | 53 |
| 1778 | Current-voltage curves for molecular junctions: pyrene vs diphenylacetylene. <i>Chemical Physics Letters</i> , 2004, 390, 246-249. | 1.2 | 19 |
| 1779 | Spin-component scaled second-order Møller-Plesset perturbation theory for the calculation of molecular geometries and harmonic vibrational frequencies. <i>Chemical Physics Letters</i> , 2004, 392, 229-235. | 1.2 | 184 |
| 1780 | A new hybrid exchange-correlation functional using the Coulomb-attenuating method (CAM-B3LYP). <i>Chemical Physics Letters</i> , 2004, 393, 51-57. | 1.2 | 11,492 |
| 1781 | Formic acid tetramers: a structural study. <i>Chemical Physics Letters</i> , 2004, 393, 347-354. | 1.2 | 27 |
| 1782 | Molecular orbital engineering of single-molecular light emission. <i>Chemical Physics Letters</i> , 2004, 394, 194-197. | 1.2 | 8 |
| 1783 | Photo-oxidation of lipids by singlet oxygen: a theoretical study. <i>Chemical Physics Letters</i> , 2004, 398, 336-342. | 1.2 | 23 |
| 1784 | Calculation of nuclear magnetic resonance shielding constants using potential-based methods. <i>Chemical Physics Letters</i> , 2004, 399, 84-88. | 1.2 | 25 |
| 1785 | A systematic study of the effect of correlation, DFT functional and basis set on the structure of Roesky's ketone. <i>Chemical Physics Letters</i> , 2004, 399, 516-521. | 1.2 | 10 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1786 | Laser-induced splittings in the nuclear magnetic resonance spectra of the rare gas atoms. <i>Chemical Physics Letters</i> , 2004, 400, 226-230. | 1.2 | 15 |
| 1787 | The triplet state of a platinum acetylide chromophore examined by time-resolved infrared spectroscopy and density functional theory. <i>Chemical Physics Letters</i> , 2004, 400, 239-244. | 1.2 | 37 |
| 1788 | The infrared spectrum of matrix isolated aminoacetonitrile, a precursor to the amino acid glycine. <i>Advances in Space Research</i> , 2004, 33, 40-43. | 1.2 | 27 |
| 1789 | Five-Coordinate FeIIINO and FeIICO Porphyrinates: Where Are the Electrons and Why Does It Matter?. <i>Journal of the American Chemical Society</i> , 2004, 126, 14136-14148. | 6.6 | 77 |
| 1790 | Re-evaluation of the Mn(salen) mediated epoxidation of alkenes by means of the B3LYP* density functional Electronic supplementary information (ESI) available: Optimised geometries, bonding energies, final gradients, spin expectation values, and imaginary frequencies for transition states. See http://www.rsc.org/suppdata/cp/b4/b402188f/ . <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 3747. | 1.3 | 28 |
| 1791 | Computational QM/MM study on the structure and energetics of species involved in the activation of the C-H and C-S bonds of thiophene by Cp*RhPMe3. <i>New Journal of Chemistry</i> , 2004, 28, 625-630. | 1.4 | 24 |
| 1792 | Electrochemical and theoretical study of the redox properties of transition metal complexes with {Pt2S2} cores. <i>Dalton Transactions</i> , 2004, , 706-712. | 1.6 | 10 |
| 1793 | Tests of second-generation and third-generation density functionals for thermochemical kinetics Electronic supplementary information (ESI) available: Mean errors for pure and hybrid DFT methods. See http://www.rsc.org/suppdata/cp/b3/b316260e/ . <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 673. | 1.3 | 242 |
| 1794 | Structural flexibility of formally d10 [M(biphosphinine)2]q complexes Electronic supplementary information (ESI) available: main geometrical parameters optimized for the structures whose energies are reported in Fig. 1. See http://www.rsc.org/suppdata/nj/b3/b316684h/ . <i>New Journal of Chemistry</i> , 2004, 28, 838. | 1.4 | 10 |
| 1795 | Fast-Flow EPR Spectroscopic Observation of the Isoniazid, Iproniazid, and Phenylhydrazine Hydrazyl Radicals. <i>Chemical Research in Toxicology</i> , 2004, 17, 226-233. | 1.7 | 14 |
| 1796 | Do the interstellar molecules CCCO and CCCS rearrange when energised?. <i>Organic and Biomolecular Chemistry</i> , 2004, 2, 999. | 1.5 | 26 |
| 1797 | Flexible N,N,N-chelates as supports for iron and cobalt chloride complexes; synthesis, structures, DFT calculations and ethylene oligomerisation studies. <i>Dalton Transactions</i> , 2004, , 3231-3240. | 1.6 | 38 |
| 1798 | A dissociative mechanism for phosphine exchange in quadruply bonded bimetallic complexes. <i>New Journal of Chemistry</i> , 2004, , . | 1.4 | 0 |
| 1799 | Multielectron Atom Transfer Reactions of Perchlorate and Other Substrates Catalyzed by Rhenium Oxazoline and Thiazoline Complexes: A Reaction Kinetics, Mechanisms, and Density Functional Theory Calculations. <i>Inorganic Chemistry</i> , 2004, 43, 4036-4050. | 1.9 | 92 |
| 1800 | Influence of Hydrogen Bonding in the Paramagnetic NMR Shieldings of Nitronyl Nitroxide Derivative Molecules. <i>Journal of Physical Chemistry B</i> , 2004, 108, 1197-1206. | 1.2 | 8 |
| 1801 | Transferable polarizabilities for the alkanes. <i>Molecular Physics</i> , 2004, 102, 985-991. | 0.8 | 12 |
| 1802 | Deuteration effects on the vibronic structure of the fluorescence spectra and the internal conversion rates of triangular [4]phenylene. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 5476-5483. | 1.3 | 13 |
| 1803 | Vibrationally resolved electronic spectroscopy and theoretical studies of deuterated 2-(2-pyridyl)indole. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 363-367. | 1.3 | 16 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1804 | Properties of WAu12. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 11-22. | 1.3 | 97 |
| 1805 | Are Hartree-Fock atoms too small or too large?. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 2928-2931. | 1.3 | 9 |
| 1806 | Establishing the NO oxidation state in complexes $[Cl_5(NO)M]^{n+}$, M = Ru or Ir, through experiments and DFT calculations. <i>Dalton Transactions</i> , 2004, , 1797-1800. | 1.6 | 52 |
| 1807 | Phytochromobilin C15-Z,syn? C15-E,anti isomerization: concerted or stepwise?. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 5066. | 1.3 | 20 |
| 1808 | Conformational dependence of the electronic absorption by astaxanthin and its implications for the bathochromic shift in crustacyanin. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 4190. | 1.3 | 25 |
| 1809 | Theoretical studies of the oxidative addition of azolium salts to a model Wilkinson's catalyst Electronic supplementary information (ESI) available: Electronic energies, zero point vibrational energies and enthalpy corrections. See http://www.rsc.org/suppdata/dt/b4/b407088g/ . <i>Dalton Transactions</i> , 2004, , 2505. | 1.6 | 20 |
| 1810 | Roesky's ketone: a spectroscopic study. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 5140-5144. | 1.3 | 12 |
| 1811 | Quantum chemical studies of dioxygen activation by mononuclear non-heme iron enzymes with the 2-His-1-carboxylate facial triad. <i>Dalton Transactions</i> , 2004, , 3153. | 1.6 | 84 |
| 1812 | $\{(1/4-L)[RuL(acac)_2]_2\}_n$, n = 2+, +, 0, \hat{a}^+ , $2\hat{a}^+$, with L = 3,3'-tetraimino-3,3'-tetrahydrobiphenyl. EPR-supported assignment of NIR absorptions for the paramagnetic intermediates. <i>Dalton Transactions</i> , 2004, , 750-753. | 1.6 | 40 |
| 1813 | Generation of transient neutrals in the gas phase from anionic precursors. Does energised CNCCO rearrange to NCCCO?. <i>Organic and Biomolecular Chemistry</i> , 2004, 2, 1742. | 1.5 | 3 |
| 1814 | Reduced and excited states of the intermediates $(\hat{1}\pm\text{-diimine})(C_5R_5)Rh$ in hydride transfer catalysis schemes: EPR and resonance Raman spectroscopy, and comparative DFT calculations of Co, Rh and Ir analogues. <i>Dalton Transactions</i> , 2004, , 3815-3821. | 1.6 | 14 |
| 1815 | Density Functional Calculations. , 2004, , 385-445. | | 0 |
| 1816 | Accurate prediction of heat of formation by combining Hartree-Fock/density functional theory calculation with linear regression correction approach. <i>Journal of Chemical Physics</i> , 2004, 121, 7086-7095. | 1.2 | 52 |
| 1817 | Curvy-steps approach to constraint-free extended-Lagrangian ab initio molecular dynamics, using atom-centered basis functions: Convergence toward Born-Oppenheimer trajectories. <i>Journal of Chemical Physics</i> , 2004, 121, 11542-11556. | 1.2 | 65 |
| 1818 | The molecular physics lecture 2004: (i) Density functional theory, (ii) Quantum Monte Carlo. <i>Molecular Physics</i> , 2004, 102, 2399-2409. | 0.8 | 36 |
| 1819 | Spin-Orbit Effects on Hyperfine Coupling Tensors in Transition Metal Complexes Using Hybrid Density Functionals and Accurate Spin-Orbit Operators. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5026-5033. | 1.1 | 62 |
| 1820 | Local Aromaticity of the Six-Membered Rings in Pyracylene. A Difficult Case for the NICS Indicator of Aromaticity. <i>Journal of Organic Chemistry</i> , 2004, 69, 7537-7542. | 1.7 | 113 |
| 1821 | Theoretical Enthalpies of Formation and O-H Bond Dissociation Enthalpy of an Ubiquinol Model and Its Free Radical. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2508-2513. | 1.1 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1822 | Quantum Mechanics Calculations on Rhodamine Dyes Require Inclusion of Solvent Water for Accurate Representation of the Structure. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7744-7751. | 1.1 | 27 |
| 1823 | Electron-Deficient Bonding in π -Rhombooid Rings. <i>Journal of the American Chemical Society</i> , 2004, 126, 13119-13131. | 6.6 | 45 |
| 1824 | Density Functional Theory Investigations on the Chemical Basis of the Selectivity Filter in the K ⁺ Channel Protein. <i>Journal of the American Chemical Society</i> , 2004, 126, 4711-4716. | 6.6 | 26 |
| 1825 | Density Functional Theory Calculations and Exploration of a Possible Mechanism of N ₂ Reduction by Nitrogenase. <i>Journal of the American Chemical Society</i> , 2004, 126, 2588-2601. | 6.6 | 98 |
| 1826 | Density Functional Theory Investigations of the Direct Oxidation of Methane on an Fe-Exchanged Zeolite. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4362-4368. | 1.2 | 45 |
| 1827 | Doubly Hybrid Meta DFT: A New Multi-Coefficient Correlation and Density Functional Methods for Thermochemistry and Thermochemical Kinetics. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4786-4791. | 1.1 | 297 |
| 1828 | Conformational Flexibility of Corey Lactone Derivatives Indicated by Absorption and Vibrational Circular Dichroism Spectra. <i>Journal of Organic Chemistry</i> , 2004, 69, 26-32. | 1.7 | 9 |
| 1829 | Computational Studies of Nucleophilic Substitution at Carbonyl Carbon: the S _N 2 Mechanism versus the Tetrahedral Intermediate in Organic Synthesis. <i>Journal of Organic Chemistry</i> , 2004, 69, 7317-7328. | 1.7 | 68 |
| 1830 | Hydrogen Bond Geometries from Electron Paramagnetic Resonance and Electron Nuclear Double Resonance Parameters: Density Functional Study of Quinone Radical Anion Solvent Interactions. <i>Journal of the American Chemical Society</i> , 2004, 126, 3280-3290. | 6.6 | 118 |
| 1831 | Comprehensive Theoretical Study of the Conversion Reactions of Spiropyrans: A Substituent and Solvent Effects. <i>Journal of Physical Chemistry B</i> , 2004, 108, 16233-16243. | 1.2 | 170 |
| 1832 | Unimolecular Decomposition of β -Hydroxyethylperoxy Radicals in the HO ₂ -Initiated Oxidation of Ethene: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11651-11663. | 1.1 | 23 |
| 1833 | Reverse Exponential Decay of Electrical Transmission in Nanosized Graphite Sheets. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7565-7572. | 1.2 | 31 |
| 1834 | Isotactic Polymers with Alternating Lactic Acid and Oxetane Subunits from the Entropically Driven Polymerization of a 14-Membered Ring. <i>Macromolecules</i> , 2004, 37, 5274-5281. | 2.2 | 24 |
| 1835 | The Generation of the Thiocyanate Radical and Cation from the Thiocyanate Anion [SCN ⁻] in the Gas Phase. The Rearrangements of Neutral and Cationic SCN. A Joint Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3668-3674. | 1.1 | 20 |
| 1836 | s-Tetrazine in Aqueous Solution: A Density Functional Study of Hydrogen Bonding and Electronic Excitations. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2044-2052. | 1.1 | 33 |
| 1837 | Preparation of Thiophene-Coordinated Ruthenium Complexes for Nonlinear Optics. <i>Organometallics</i> , 2004, 23, 1875-1879. | 1.1 | 17 |
| 1838 | Infrared Spectra of Thallium Hydrides in Solid Neon, Hydrogen, and Argon. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3396-3402. | 1.1 | 32 |
| 1839 | The Coupling Character of Ca ²⁺ with Glutamic Acid: Implication for the Conformational Behavior and Transformation of Ca ²⁺ -ATPase in Transmembrane Ca ²⁺ Channel. <i>Journal of Physical Chemistry B</i> , 2004, 108, 17628-17638. | 1.2 | 14 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1840 | Density Functional Theory Calculations of Vibrational Absorption and Circular Dichroism Spectra of Dimethyl-l-tartrate. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4080-4086. | 1.1 | 35 |
| 1841 | Reaction of Benzene and Boron Atom: Mechanism of Formation of Benzoborirene and Hydrogen Atom. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4576-4586. | 1.1 | 31 |
| 1842 | The Formation of Cyanoketene (NCCHCO) and the Isomer NCCCHO from Anionic Precursors in the Gas Phase. The Rearrangement of NCCCHO to NCCHCO. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3994-4001. | 1.1 | 8 |
| 1843 | Hydrogen Transfer between Ligands: A Density Functional Study of the Rearrangement of $M(\eta^6\text{-C}_7\text{H}_8)_2$ into $M(\eta^7\text{-C}_7\text{H}_7)(\eta^5\text{-C}_7\text{H}_9)$ [$M = \text{Mo}, \text{Mo}^+, \text{Zr}$]. <i>Organometallics</i> , 2004, 23, 2658-2669. | 1.1 | 8 |
| 1844 | Exploring Hydration Patterns of Aldehydes and Amides: Ab Initio Investigations. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2492-2498. | 1.1 | 41 |
| 1845 | Resonance Energies of the Allyl Cation and Allyl Anion: Contribution by Resonance and Inductive Effects toward the Acidity and Hydride Abstraction Enthalpy of Propene. <i>Journal of Organic Chemistry</i> , 2004, 69, 648-654. | 1.7 | 23 |
| 1846 | Deprotonation of Lithiated Benzenes. <i>Journal of Organic Chemistry</i> , 2004, 69, 2111-2122. | 1.7 | 13 |
| 1847 | Toward a Computational Description of Nitrile Hydratase: Studies of the Ground State Bonding and Spin-Dependent Energetics of Mononuclear, Non-Heme Fe(III) Complexes. <i>Inorganic Chemistry</i> , 2004, 43, 458-472. | 1.9 | 31 |
| 1848 | Performance of Density Functionals for Calculating Barrier Heights of Chemical Reactions Relevant to Astrophysics. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7621-7636. | 1.1 | 80 |
| 1849 | Wire-Length Dependence of the Conductance of Oligo(p-phenylene) Dithiolate Wires: A Consideration from Molecular Orbitals. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9143-9149. | 1.1 | 66 |
| 1850 | Density Functional Study on the Mechanisms of the Reactions of Gas-Phase OsO_n^+ ($n = 1-4$) with Methane. <i>Organometallics</i> , 2004, 23, 3656-3667. | 1.1 | 27 |
| 1851 | Excited-State Characters and Dynamics of $[\text{W}(\text{CO})_5(4\text{-cyanopyridine})]$ and $[\text{W}(\text{CO})_5(\text{piperidine})]$ Studied by Picosecond Time-Resolved IR and Resonance Raman Spectroscopy and DFT Calculations: Roles of $\text{W} \rightarrow \text{L}$ and $\text{W} \rightarrow \text{CO}$ MLCT and LF Excited States Revised. <i>Inorganic Chemistry</i> , 2004, 43, 1723-1734. | 1.9 | 31 |
| 1852 | Hydration of the Fluoride Anion: Structures and Absolute Hydration Free Energy from First-Principles Electronic Structure Calculations. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2020-2029. | 1.1 | 166 |
| 1853 | Photochemical Reaction Mechanisms of 2-Nitrobenzyl Compounds: Methyl Ethers and Caged ATP. <i>Journal of the American Chemical Society</i> , 2004, 126, 4581-4595. | 6.6 | 308 |
| 1854 | The Performance of the Handy/Cohen Functionals, OLYP and O3LYP, for the Computation of Hydrocarbon Pericyclic Reaction Activation Barriers. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2959-2965. | 1.1 | 54 |
| 1855 | The Unexpected Preference for the fac-Isomer with the Tris(5-ester-substituted-2,2'-bipyridine) Complexes of Ruthenium(II). <i>Inorganic Chemistry</i> , 2004, 43, 1714-1722. | 1.9 | 21 |
| 1856 | Coupling Character between Imidazole and Imidazole Cation: Implication for the Coupling Modes of Biomolecular Residues. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7038-7049. | 1.1 | 36 |
| 1857 | Is the Enthalpy of Fusion of Tris(acetylacetonato)metal(III) Complexes Affected by Their Potential Energy in the Crystal State?. <i>Inorganic Chemistry</i> , 2004, 43, 8479-8489. | 1.9 | 24 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1858 | Quasi-Relativistic Density Functional Study of Auophilic Interactions. <i>Journal of the American Chemical Society</i> , 2004, 126, 1266-1276. | 6.6 | 87 |
| 1859 | Density Functional Theory Study on the Initial Step of the Permanganate Oxidation of Substituted Alkynes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4455-4458. | 1.1 | 12 |
| 1860 | Density Functional Theory Studies on Structure, Spectra, and Electronic Properties of 3,7-Dinitrodibenzobromolium Cation and Chloride. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7596-7602. | 1.1 | 1 |
| 1861 | Characterization of 5-Hydroxy-8-oxo-7,8-dihydroguanosine in the Photosensitized Oxidation of 8-Oxo-7,8-dihydroguanosine and Its Rearrangement to Spiroiminodihydantoin. <i>Journal of the American Chemical Society</i> , 2004, 126, 16777-16782. | 6.6 | 80 |
| 1862 | A Quantum Chemical Study of Cu ²⁺ Interacting with Guanine-Cytosine Base Pair. Electrostatic and Oxidative Effects on Intermolecular Proton-Transfer Processes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 333-341. | 1.1 | 106 |
| 1863 | Why Are Olefins Oxidized by RuO ₄ under Cleavage of the Carbon-Carbon Bond whereas Oxidation by OsO ₄ Yields cis-Diols? <i>Journal of the American Chemical Society</i> , 2004, 126, 3642-3652. | 6.6 | 58 |
| 1864 | Structure, Bonding, and Solvation of Dilithiodiamines. <i>Journal of Organic Chemistry</i> , 2004, 69, 7519-7524. | 1.7 | 21 |
| 1865 | Use of Computational and Synthetic Chemistry in Catalyst Design: A New Family of High-Activity Ethylene Polymerization Catalysts Based on Titanium Tris(amino)phosphinimide Complexes. <i>Organometallics</i> , 2004, 23, 5240-5251. | 1.1 | 38 |
| 1866 | The Crystalline Enol of 1,3-Cyclohexanedione and Its Complex with Benzene: % Vibrational Spectra, Simulation of Structure and Dynamics and Evidence for Cooperative Hydrogen Bonding. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7356-7363. | 1.1 | 14 |
| 1867 | Comparative Study of Diastereoisomer Interconversion in Chiral BINOL-ate and Diamine Platinum Complexes of Conformationally Flexible NUPHOS Diphosphines. <i>Organometallics</i> , 2004, 23, 1055-1064. | 1.1 | 24 |
| 1868 | Oxygen Activation by Rieske Non-Heme Iron Oxygenases, a Theoretical Insight. <i>Journal of Physical Chemistry B</i> , 2004, 108, 13031-13041. | 1.2 | 27 |
| 1869 | New Universal Solvation Model and Comparison of the Accuracy of the SM5.42R, SM5.43R, C-PCM, D-PCM, and IEF-PCM Continuum Solvation Models for Aqueous and Organic Solvation Free Energies and for Vapor Pressures. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6532-6542. | 1.1 | 100 |
| 1870 | Synthesis and Characterization of Bis(di-2-pyridylmethanamine)ruthenium(II). <i>Inorganic Chemistry</i> , 2004, 43, 1735-1742. | 1.9 | 28 |
| 1871 | VIS/NIR Absorption Spectra of Positively Charged Oligo(phenylenevinylene)s and Comparison with Time-Dependent Density Functional Theory Calculations. <i>Journal of Physical Chemistry B</i> , 2004, 108, 19967-19975. | 1.2 | 13 |
| 1872 | Radiation-Induced Damage in Serine Phosphate: Insights into a Mechanism for Direct DNA Strand Breakage. <i>Journal of Physical Chemistry B</i> , 2004, 108, 8036-8042. | 1.2 | 12 |
| 1873 | H Atom and H ₂ Elimination from Y + C ₂ H ₂ . <i>Journal of Physical Chemistry A</i> , 2004, 108, 10165-10172. | 1.1 | 14 |
| 1874 | Effects of Finite Carbon Nanotube Length on Sidewall Addition of Fluorine Atom and Methylene. <i>Organic Letters</i> , 2004, 6, 731-734. | 2.4 | 69 |
| 1875 | Complex Reduction Chemistry of (abpy)PtCl ₂ , abpy = 2,2'-Azobispyridine: Formation of Cyclic [(1/4,1/2:1/1-abpy)PtCl] ²⁺ with a New Coordination Mode for abpy and a Near-Infrared Ligand-to-Ligand Intervalence Charge Transfer Absorption of the One-Electron Reduced State. <i>Inorganic Chemistry</i> , 2004, 43, 5973-5980. | 1.9 | 72 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1876 | The Reaction of Cyclopentyne with Ethene: A Concerted vs Stepwise Mechanism?. <i>Journal of Organic Chemistry</i> , 2004, 69, 6357-6364. | 1.7 | 40 |
| 1877 | Functionalization of Carbon Nanotubes by Ammonia Glow-Discharge: A % Experiments and Modeling. <i>Journal of Physical Chemistry B</i> , 2004, 108, 8166-8172. | 1.2 | 97 |
| 1878 | Model Studies on p-Hydroxybenzoate Hydroxylase. The Catalytic Role of Arg-214 and Tyr-201 in the Hydroxylation Step. <i>Journal of the American Chemical Society</i> , 2004, 126, 127-142. | 6.6 | 11 |
| 1879 | Alcoholysis of N-Methyl-1,2-Thiazetidine-1,1-Dioxide: A DFT Study of Water and Alcohol Effects. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7702-7708. | 1.1 | 13 |
| 1880 | Assessment of Handy's Cohen Optimized Exchange Density Functional (OPTX). <i>Journal of Physical Chemistry A</i> , 2004, 108, 8495-8504. | 1.1 | 51 |
| 1881 | Radical-Like Activation of Alkanes by the Ligated Copper Oxide Cation (Phenanthroline)CuO+. <i>Journal of Physical Chemistry B</i> , 2004, 108, 14407-14416. | 1.2 | 134 |
| 1882 | A Density Functional Theory Study on the Adsorption of Chlorobenzene on the Si(111)-7 Å ² Surface. <i>Journal of Physical Chemistry B</i> , 2004, 108, 14049-14055. | 1.2 | 16 |
| 1883 | Direct Observation of the Forbidden Hydrogen Atom Adduct to Acetonitrile: A Neutralization-Reionization Mass Spectrometric and CCSD(T) ab Initio/RRKM Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4163-4173. | 1.1 | 11 |
| 1884 | Ion Chemistry of OV(OCH ₃) ₃ in the Gas Phase: A Molecular Cations and Anions and Their Primary Fragmentations. <i>Inorganic Chemistry</i> , 2004, 43, 1976-1985. | 1.9 | 31 |
| 1885 | Reduction Mechanisms of Ethylene, Propylene, and Vinylethylene Carbonates. <i>Journal of the Electrochemical Society</i> , 2004, 151, A178. | 1.3 | 181 |
| 1886 | Arene Hapticity in (C ₆ H ₆)Cr(CO) _n (n = 1-5) Complexes: A DFT Study of Singlet and Triplet Energy Surfaces. <i>Organometallics</i> , 2004, 23, 2315-2325. | 1.1 | 24 |
| 1887 | Evidence for Discrepancy between the Surface Lewis Acid Site Strength and Infrared Spectra of Adsorbed Molecules: The Case of Boric Acid on Silica. <i>Journal of Physical Chemistry B</i> , 2004, 108, 16499-16507. | 1.2 | 24 |
| 1888 | Vibrational Frequencies of Amides and Amide Dimers: The Assessment of PW91XC Functional. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7291-7300. | 1.1 | 33 |
| 1889 | Influence of the Cis Ligand on the H-H Separation and the Rotation Barrier of the Dihydrogen in Osmium-Elongated Dihydrogen Complexes Containing an Ortho-Metalated Ketone. <i>Organometallics</i> , 2004, 23, 3008-3015. | 1.1 | 48 |
| 1890 | Creation of Hoop- and Bowl-Shaped Benzenoid Systems by Selective Detraction of [60]Fullerene Conjugation. [10]Cyclophenacene and Fused Corannulene Derivatives. <i>Journal of the American Chemical Society</i> , 2004, 126, 8725-8734. | 6.6 | 84 |
| 1891 | Rapid Quantum Mechanical Models for the Computational Estimation of C-H Bond Dissociation Energies as a Measure of Metabolic Stability. <i>Molecular Pharmaceutics</i> , 2004, 1, 128-135. | 2.3 | 16 |
| 1892 | Reassessment of the Level of Theory Required for the Epoxidation of Ethylene with Dioxiranes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6886-6892. | 1.1 | 19 |
| 1893 | Molecular Modeling of Environmentally Important Processes: Reduction Potentials. <i>Journal of Chemical Education</i> , 2004, 81, 596. | 1.1 | 150 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1894 | Validation of Theoretical Methods for the Structure and Energy of Aluminum Clusters. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4850-4861. | 1.2 | 72 |
| 1895 | Chiroptical Properties of Some Monoazapentahelicenes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11752-11761. | 1.1 | 29 |
| 1896 | Infrared Spectra of Indium Hydrides in Solid Hydrogen and Neon. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4440-4448. | 1.1 | 26 |
| 1897 | Mechanistic Details of Nickel(0)-Assisted Oxidative Coupling of CO ₂ with C ₂ H ₄ . <i>Organometallics</i> , 2004, 23, 5252-5259. | 1.1 | 95 |
| 1898 | Chromogenic and Neurotoxic Effects of an Aliphatic β^3 -Diketone: Computational Insights into the Molecular Structures and Mechanism. <i>Journal of Physical Chemistry B</i> , 2004, 108, 6098-6104. | 1.2 | 18 |
| 1899 | Combined Raman and Computational Study of a Novel Series of Macrocyclic π -Conjugated Diacetylene-Bridged β^{\pm} -Linked Oligothiophenes. <i>Journal of Physical Chemistry B</i> , 2004, 108, 3158-3167. | 1.2 | 24 |
| 1900 | Low Energy Dissociation Processes of Ionized Cyclohexene: A Theoretical Insight. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9853-9862. | 1.1 | 10 |
| 1901 | Ultrafast Photochemical Dissociation of an Equatorial CO Ligand from $\text{trans}(X,X)\text{-[Ru}(X)_2(\text{CO})_2(\text{bpy})]$ (X = Cl, Br, I): A Picosecond Time-Resolved Infrared Spectroscopic and DFT Computational Study. <i>Inorganic Chemistry</i> , 2004, 43, 7380-7388. | 1.9 | 52 |
| 1902 | A Molecular Orbital Study of Tambjamine E and Analogues. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4542-4550. | 1.1 | 1 |
| 1903 | What is the Ground State of Ni(O ₂)? <i>Journal of Physical Chemistry A</i> , 2004, 108, 2871-2873. | 1.1 | 13 |
| 1904 | Structure and Dynamics of Neutral β^2 -H Agostic Nickel Alkyls: A Combined Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2004, 126, 11984-11994. | 6.6 | 76 |
| 1905 | Binding of NH ₃ to graphite and to a (9,0) carbon nanotube. <i>Physical Review B</i> , 2004, 70, . | 1.1 | 83 |
| 1906 | Activation of Methane by MH ⁺ (M = Fe, Co, and Ni): A Combined Mass Spectrometric and DFT Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9755-9761. | 1.1 | 66 |
| 1907 | Determination of absolute configuration via vibrational circular dichroism. <i>Drug Discovery Today: Technologies</i> , 2004, 1, 269-275. | 4.0 | 30 |
| 1908 | Binding of propene on small gold clusters and on Au(111): Simple rules for binding sites and relative binding energies. <i>Journal of Chemical Physics</i> , 2004, 121, 3756-3766. | 1.2 | 94 |
| 1909 | Meta-generalized gradient approximation: Explanation of a realistic nonempirical density functional. <i>Journal of Chemical Physics</i> , 2004, 120, 6898-6911. | 1.2 | 431 |
| 1910 | Molecular Geometry as a Source of Chemical Information. 3. How H-Bonding Affects Aromaticity of the Ring in the Case of Phenol and p-Nitrophenol Complexes: A B3LYP/6-311+G** Study. <i>Journal of Organic Chemistry</i> , 2004, 69, 7038-7043. | 1.7 | 41 |
| 1911 | Isotope effect on the Jahn-T distortion of partially deuteriated benzene cation radicals: an experimental EPR and theoretical DFT study. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 1658-1665. | 1.3 | 6 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1912 | A Comparative Study of Overtone CH-Stretching Vibrational Circular Dichroism Spectra of Fenchone and Camphor. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5338-5352. | 1.1 | 29 |
| 1913 | Hybrid Meta Density Functional Theory Methods for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions: The MPW1B95 and MPWB1K Models and Comparative Assessments for Hydrogen Bonding and van der Waals Interactions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6908-6918. | 1.1 | 1,497 |
| 1914 | Ground and Low-Lying States of $\text{Cu}^{2+}\text{H}_2\text{O}$. A Difficult Case for Density Functional Methods. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6072-6078. | 1.1 | 85 |
| 1915 | Conformational Effects on the Optical Rotation of Alanine and Proline. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4269-4276. | 1.1 | 103 |
| 1916 | Performance of the OPBE exchange-correlation functional. <i>Molecular Physics</i> , 2004, 102, 2467-2474. | 0.8 | 378 |
| 1917 | Quantum Chemistry Study of Actinide(III) and Lanthanide(III) Complexes with Tridentate Nitrogen Ligands. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6893-6900. | 1.1 | 106 |
| 1918 | Modeling vibrational spectra using the self-consistent charge density-functional tight-binding method. I. Raman spectra. <i>Journal of Chemical Physics</i> , 2004, 121, 5171-5178. | 1.2 | 46 |
| 1919 | Electronic Modulation of Dithienothiophene (DTT) as π -Center of D- π -D Chromophores on Optical and Redox Properties: A Analysis by UV-Vis-NIR and Raman Spectroscopies Combined with Electrochemistry and Quantum Chemical DFT Calculations. <i>Journal of the American Chemical Society</i> , 2004, 126, 13363-13376. | 6.6 | 52 |
| 1920 | Density Functional Study of Ammonia Activation by Late First-Row Transition Metal Cations. <i>Inorganic Chemistry</i> , 2004, 43, 4944-4952. | 1.9 | 37 |
| 1921 | Distonic Isomers and Tautomers of the Adenine Cation Radical in the Gas Phase and Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9283-9293. | 1.1 | 46 |
| 1922 | The Role of Fullerene Hemispheres in Determining Structural Features of Finite-Length Carbon Nanotubes. <i>Journal of Physical Chemistry B</i> , 2004, 108, 11426-11434. | 1.2 | 49 |
| 1923 | Accurate Energies and Structures for Large Water Clusters Using the X3LYP Hybrid Density Functional. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10518-10526. | 1.1 | 134 |
| 1924 | TD-DFT Computational Insight into the Origin of Wavelength-Dependent E/Z Photoisomerization of Urocanic Acid. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5662-5669. | 1.1 | 11 |
| 1925 | Theoretical Investigations of the Electronic Structure and Spectroscopy of Mononuclear, Non-Heme $\{\text{Fe}(\text{NO})_6\}$ Complexes. <i>Inorganic Chemistry</i> , 2004, 43, 7030-7041. | 1.9 | 35 |
| 1926 | First principles electrochemical study of redox events in DNA bases and chemical repair in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 2426. | 1.3 | 20 |
| 1927 | Catalyzed Chemoselective Acrolein Hydrogenation. Density Functional Studies. <i>Organometallics</i> , 2004, 23, 2168-2178. | 1.1 | 14 |
| 1928 | Structure and Coordination Modes in the Interaction between Cd^{2+} and 3-Mercaptopropionic Acid. <i>Journal of Physical Chemistry A</i> , 2004, 108, 8407-8410. | 1.1 | 17 |
| 1929 | Experimental and Numerical Studies of Ethanol Decomposition Reactions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7671-7680. | 1.1 | 155 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1930 | Thermochemical Properties, Pathway, and Kinetic Analysis on the Reactions of Benzene with OH: An Elementary Reaction Mechanism. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4632-4652. | 1.1 | 49 |
| 1931 | Potential Energy and Spin-Spin Coupling Constants Surface of Glycolaldehyde. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2758-2769. | 1.1 | 18 |
| 1932 | Photoelectron Spectroscopy of Free Polyoxoanions Mo ₆ O ₁₉ ²⁻ and W ₆ O ₁₉ ²⁻ in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10089-10093. | 1.1 | 54 |
| 1933 | Calculating the Electron Paramagnetic Resonance Parameters of Exchange Coupled Transition Metal Complexes Using Broken Symmetry Density Functional Theory: Application to a Mn ^{III} /Mn ^{IV} Model Compound. <i>Journal of the American Chemical Society</i> , 2004, 126, 2613-2622. | 6.6 | 194 |
| 1934 | Competition between linear and cyclic structures in monochromium carbide clusters CrC _n ⁺ and CrC _n ⁻ (n=2-8): A photoelectron spectroscopy and density functional study. <i>Journal of Chemical Physics</i> , 2004, 120, 8996-9008. | 1.2 | 64 |
| 1935 | Icosahedral gold cage clusters: M@Au ₁₂ ⁺ (M=V, Nb, and Ta). <i>Journal of Chemical Physics</i> , 2004, 121, 8369. | 1.2 | 137 |
| 1936 | Discrepancy between common local aromaticity measures in a series of carbazole derivatives. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 314-318. | 1.3 | 106 |
| 1937 | Photosensitized Reactions of Oxime Ethers: A Steady-State and Laser Flash Photolysis Study. <i>Journal of Organic Chemistry</i> , 2004, 69, 3057-3067. | 1.7 | 26 |
| 1938 | Supported metal species and adsorption complexes on metal oxides and in zeolites: Density functional cluster model studies. <i>Theoretical and Computational Chemistry</i> , 2004, , 367-450. | 0.2 | 5 |
| 1939 | Excited State Potentials and Ligand Force Field of a Blue Copper Protein Plastocyanin. <i>Journal of Physical Chemistry B</i> , 2004, 108, 3940-3946. | 1.2 | 24 |
| 1940 | Nucleophilic Attack at Selenium in Diselenides and Selenosulfides. A Computational Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4040-4046. | 1.1 | 85 |
| 1941 | Combined Quantum Chemical/RRKM-ME Computational Study of the Phenyl + Ethylene, Vinyl + Benzene, and H + Styrene Reactions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9697-9714. | 1.1 | 50 |
| 1942 | Effect of the Perdew-Zunger self-interaction correction on the thermochemical performance of approximate density functionals. <i>Journal of Chemical Physics</i> , 2004, 121, 8187. | 1.2 | 147 |
| 1943 | Synthesis of [(MeCyt) ₂ H] ⁺ structure and stability of a dimeric threefold hydrogen-bonded 1-methylcytosinium 1-methylcytosine cation. <i>Organic and Biomolecular Chemistry</i> , 2004, 2, 2513-2516. | 1.5 | 14 |
| 1944 | Combined Spectroscopic and Theoretical Study of Narrow Band Gap Heterocyclic Co-oligomers Containing Alternating Aromatic Donor and Quinoid Acceptor Units. <i>Journal of Physical Chemistry B</i> , 2004, 108, 2516-2526. | 1.2 | 66 |
| 1945 | Ab Initio Quantum Chemical and Molecular Dynamics Simulation Study of Lithium Iodide in Acetonitrile. <i>Zeitschrift Fur Physikalische Chemie</i> , 2004, 218, 643-658. | 1.4 | 8 |
| 1946 | An ab initio study of structural properties and single vacancy defects in Wurtzite AlN. <i>Journal of Chemical Physics</i> , 2004, 120, 4890-4896. | 1.2 | 31 |
| 1947 | Linear-scaling formation of Kohn-Sham Hamiltonian: Application to the calculation of excitation energies and polarizabilities of large molecular systems. <i>Journal of Chemical Physics</i> , 2004, 121, 2915-2931. | 1.2 | 52 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1948 | N-benzoylimido complexes of palladium. Synthesis, structural characterisation and structureâ€“reactivity relationship. Dalton Transactions, 2004, , 2041-2050. | 1.6 | 7 |
| 1949 | Tests of a ladder of density functionals for bulk solids and surfaces. Physical Review B, 2004, 69, . | 1.1 | 349 |
| 1950 | Density-functional generalized-gradient and hybrid calculations of electromagnetic properties using Slater basis sets. Journal of Chemical Physics, 2004, 120, 7252-7261. | 1.2 | 28 |
| 1951 | Theoretical calculations of infrared absorption, vibrational circular dichroism, and two-dimensional vibrational spectra of acetylproline in liquids water and chloroform. Journal of Chemical Physics, 2004, 121, 1849-1865. | 1.2 | 43 |
| 1952 | Development and Assessment of a New Hybrid Density Functional Model for Thermochemical Kinetics. Journal of Physical Chemistry A, 2004, 108, 2715-2719. | 1.1 | 639 |
| 1953 | DFT study of conjugated biheterocyclic oligomers exhibiting a very low HOMOâ€“LUMO energy gap. Synthetic Metals, 2004, 140, 127-133. | 2.1 | 24 |
| 1954 | The Stability of documentclass{aastex} usepackage{amssymb} usepackage{amsmath} usepackage{amsxtra} usepackage{amsthm} usepackage{amsfonts} usepackage{amscd} usepackage{amstext} usepackage{amsbsy} usepackage{amsfonts} usepackage{amssymb} usepackage{bm} usepackage{mathrsfs} usepackage{pifont} usepackage{stmaryrd} usepackage{textcomp} usepackage{portland,xspace} usepackage{amsmath,amsxtra} usepackage[OT2,OT1]{fontenc} ewcommandcyr{enewcommandmdefault{wncyr} anewcommandsfdefault{wncyss} anewcommandencodingdefault{OT2} ormalfont selectfont} DeclareTextFontCommand{extcyr} | 1.6 | 23 |
| 1955 | The Impact of Deuteration on the Infrared Spectra of Interstellar Polycyclic Aromatic Hydrocarbons. Astrophysical Journal, 2004, 614, 770-780. | 1.6 | 29 |
| 1956 | Extended Barbaralanes:Â Sigmotropic Shiftamers or Îf-Polyacenes?. Journal of the American Chemical Society, 2004, 126, 4256-4263. | 6.6 | 26 |
| 1957 | A Theoretical Study of the Ring-Opening of Metallacyclobutene Derived from the Addition of Acetylene to Molybdenum Alkylidenes. Organometallics, 2004, 23, 3189-3196. | 1.1 | 10 |
| 1958 | QUANTUM CHEMICAL INVESTIGATIONS INTO THE PROBLEM OF BIOLOGICAL NITROGEN FIXATION: SELLMANN-TYPE METALâ€“SULFUR MODEL COMPLEXES. Advances in Inorganic Chemistry, 2004, , 55-100. | 0.4 | 14 |
| 1959 | A Vibrational Analysis on Possible Peroxo Forms of Soluble Methane Monooxygenase. Bulletin of the Chemical Society of Japan, 2004, 77, 1305-1311. | 2.0 | 12 |
| 1960 | Electron-Rich Radicals by Neutralizationâ€“Reionization Mass Spectrometry. Generation, Dissociations and Energetics of the Hydrogen Atom Adduct to Acetamide. European Journal of Mass Spectrometry, 2004, 10, 869-879. | 0.5 | 7 |
| 1961 | The Gas-Phase Rearrangement of HCCBCCH to a Trans Pentacyclic Isomer. A Joint Experimental and Theoretical Study. European Journal of Mass Spectrometry, 2004, 10, 829-835. | 0.5 | 3 |
| 1962 | Rearrangements of Transient Neutral Molecules in the Gas Phase. Does the Conversion of CCCHO to HCCCO Involve Oxygen or Hydrogen Migration?. European Journal of Mass Spectrometry, 2004, 10, 441-448. | 0.5 | 2 |
| 1963 | Ring Complexes of S-Nitrosothiols with Cu+: A Density Functional Theory Study. European Journal of Mass Spectrometry, 2004, 10, 941-948. | 0.5 | 4 |
| 1964 | Electronic absorption spectra of PAHs up to vacuum UV. Astronomy and Astrophysics, 2004, 426, 105-117. | 2.1 | 112 |
| 1965 | Tautomerization in the ground and first excited singlet states of phenyl-lapimidazole. Journal of Luminescence, 2004, 109, 207-214. | 1.5 | 2 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 1966 | Probing Shapes of Bichromophoric Metal-Organic Complexes Using Ion Mobility Mass Spectrometry. <i>Journal of the American Chemical Society</i> , 2005, 127, 18222-18228. | 6.6 | 23 |
| 1967 | End-Cap Effects on Vibrational Structures of Finite-Length Carbon Nanotubes. <i>Journal of the American Chemical Society</i> , 2005, 127, 11769-11776. | 6.6 | 59 |
| 1969 | Scalable molecular dynamics. <i>Journal of Physics: Conference Series</i> , 2005, 16, 287-299. | 0.3 | 3 |
| 1971 | A Computational Study of Lithium Dialkylamide Mixed Aggregates with Lithium Chloride. <i>Bulletin of the Chemical Society of Japan</i> , 2005, 78, 890-898. | 2.0 | 25 |
| 1972 | Principal Component Analysis with Energy Density of Calophyllum Coumarins. <i>Chemistry Letters</i> , 2005, 34, 844-845. | 0.7 | 11 |
| 1973 | Infrared spectroscopy of matrix-isolated polycyclic aromatic compounds and their ions. 7. Phenazine, a dual substituted polycyclic aromatic nitrogen heterocycle. <i>Advances in Space Research</i> , 2005, 36, 156-165. | 1.2 | 27 |
| 1974 | A high-resolution infrared study of five bands of 1,2,5-thiadiazole in the range 750-1250 cm ⁻¹ , together with ab initio and DFT studies. <i>Journal of Molecular Spectroscopy</i> , 2005, 233, 256-268. | 0.4 | 14 |
| 1975 | Synthesis, characterization and Schlenk equilibrium studies of methylmagnesium compounds with O- and N-donor ligands – the unexpected behavior of [MgMeBr(pmdta)] (pmdta=N,N,N,N-tetramethylethylenetriamine). <i>Journal of Organometallic Chemistry</i> , 2005, 690, 1178-1191. | 0.8 | 31 |
| 1976 | Synthesis, structure and optical limiting properties of organoruthenium chalcogenide clusters. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 1487-1497. | 0.8 | 19 |
| 1977 | Mechanistic studies on the formation of Pt(II) hydroformylation catalysts in imidazolium-based ionic liquids. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 3567-3576. | 0.8 | 94 |
| 1978 | Reactivity of the dinuclear platinum-diketone [Pt ₂ {(COMe) ₂ H} ₂ (I ^{1/4} -Cl) ₂] towards chelating ligands – Bridge cleavage versus formation of acetyl(chloro)platinum(II) complexes. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 3229-3236. | 0.8 | 15 |
| 1979 | Replacement of N-heterocyclic carbenes by N-heterocyclic silylenes at a Pd(0) center: Experiment and theory. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 3292-3299. | 0.8 | 25 |
| 1980 | Chemical bonding in transition metal carbene complexes. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 6178-6204. | 0.8 | 206 |
| 1981 | Theoretical study of the photoinduced intramolecular proton transfer and rotational processes in 2-(2-hydroxyphenyl)-4-methyl-5-oxazolone in gas phase and embedded in β -cyclodextrin. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2005, 173, 365-374. | 2.0 | 17 |
| 1982 | Theoretical study on excitation dynamics of 5-dibenzosuberone and its derivatives. <i>Journal of Molecular Structure</i> , 2005, 735-736, 211-216. | 1.8 | 1 |
| 1983 | Complexes of dibromo(ethylenediamine)-palladium(II) observed from aqueous solutions by electrospray mass spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2005, 16, 1461-1469. | 1.2 | 21 |
| 1984 | Experimental and theoretical investigations of the loss of amino acid side chains in electron capture dissociation of model peptides. <i>Journal of the American Society for Mass Spectrometry</i> , 2005, 16, 1523-1535. | 1.2 | 89 |
| 1985 | Cyclization reactions of acylium and thioacylium ions with isocyanates and isothiocyanates: Gas phase synthesis of 3,4-dihydro-2,4-dioxo-2H-1,3,5-oxadiazinium ions. <i>Journal of the American Society for Mass Spectrometry</i> , 2005, 16, 1602-1607. | 1.2 | 7 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 1986 | Protonated adenine: Tautomers, solvated clusters, and dissociation mechanisms. <i>Journal of the American Society for Mass Spectrometry</i> , 2005, 16, 1713-1726. | 1.2 | 69 |
| 1987 | Simple b ions have cyclic oxazolone structures. A neutralization-reionization mass spectrometric and computational study of oxazolone radicals. <i>Journal of the American Society for Mass Spectrometry</i> , 2005, 16, 1941-1956. | 1.2 | 28 |
| 1988 | Cation templation of $Mn^{2+}/[Mo(CN)_7]^{4-}$ system: Formation of pseudo-dimorphs $(NH_4)_2Mn_3(H_2O)_4[Mo(CN)_7]_2 \cdot nH_2O$ ($n=4, 5$). <i>Polyhedron</i> , 2005, 24, 1033-1046. | 1.0 | 5 |
| 1989 | Theoretical methods that help understanding the structure and reactivity of gas phase ions. <i>International Journal of Mass Spectrometry</i> , 2005, 240, 37-99. | 0.7 | 104 |
| 1990 | The aluminum phosphides $AlmP_n$ ($m+n=2 \leq 5$) and their anions: structures, electron affinities and vibrational frequencies. <i>International Journal of Mass Spectrometry</i> , 2005, 240, 149-159. | 0.7 | 15 |
| 1991 | Binding interactions of mono- and diatomic silver cations with small alkenes: experiment and theory. <i>International Journal of Mass Spectrometry</i> , 2005, 241, 109-117. | 0.7 | 36 |
| 1992 | One-pot synthesis of the macroporous polyaniline microspheres and Ag/polyaniline core-shell particles. <i>Microporous and Mesoporous Materials</i> , 2005, 84, 254-260. | 2.2 | 53 |
| 1993 | Quantum and molecular mechanics calculations on modified silica nano ring. <i>Journal of Molecular Structure</i> , 2005, 739, 163-172. | 1.8 | 10 |
| 1994 | An experimental and theoretical study on the states of PHBA in aqueous solution. <i>Journal of Molecular Structure</i> , 2005, 752, 198-202. | 1.8 | 5 |
| 1995 | Synthesis and characterization of azole isoflavone inhibitors of aromatase. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 4063-4070. | 1.4 | 35 |
| 1996 | Pentamers of formic acid. <i>Chemical Physics</i> , 2005, 312, 119-126. | 0.9 | 26 |
| 1997 | Influence of (S)-1-phenylethylamine para substitution on the resolution of (Δ ±)-1,4-benzodioxane-2-carboxylic acid: a crystallographic, theoretical and morphologic approach. <i>Tetrahedron: Asymmetry</i> , 2005, 16, 2099-2106. | 1.8 | 16 |
| 1998 | Evidence for a nucleophilic anti-attack on the cleaved C(2)-oxygen bond in Cl_2AlH -catalyzed ring-opening of 2-substituted 1,3-dioxolanes. <i>Tetrahedron Letters</i> , 2005, 46, 1837-1840. | 0.7 | 9 |
| 1999 | 1,3-Dipolar cycloaddition of azomethine ylide with ethene and 2-butene: a computational study. <i>Tetrahedron Letters</i> , 2005, 46, 1993-1995. | 0.7 | 8 |
| 2000 | Synthesis and photoluminescence study of benz[<i>f</i>]indene derivatives. <i>Tetrahedron Letters</i> , 2005, 46, 4627-4631. | 0.7 | 10 |
| 2001 | Synthesis and properties of novel guanidine bases. N,N,N'-Tris(3-dimethylaminopropyl)-guanidine. <i>Tetrahedron Letters</i> , 2005, 46, 8733-8736. | 0.7 | 39 |
| 2002 | Structure of functionalized porous metal-organic frameworks by molecular orbital methods. <i>Computational and Theoretical Chemistry</i> , 2005, 716, 33-38. | 1.5 | 12 |
| 2003 | Spectroscopic properties of molecular anions of astrophysical and laboratory interest. <i>Computational and Theoretical Chemistry</i> , 2005, 713, 101-106. | 1.5 | 6 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2004 | Theoretical enthalpies of formation for atmospheric hydroxycarbonyls. Computational and Theoretical Chemistry, 2005, 713, 119-125. | 1.5 | 12 |
| 2005 | Theoretical study of aryl succinic and maleic acid derivatives. Computational and Theoretical Chemistry, 2005, 713, 127-134. | 1.5 | 10 |
| 2006 | Nitric acid dimers. Computational and Theoretical Chemistry, 2005, 714, 217-220. | 1.5 | 9 |
| 2007 | Vibrational spectra of phthalazine by density functional theory calculations and assignment of its metal complexes. Computational and Theoretical Chemistry, 2005, 717, 171-178. | 1.5 | 6 |
| 2008 | Prediction of gas phase thermodynamic properties of polychlorinated dibenzo-furans by DFT. Computational and Theoretical Chemistry, 2005, 725, 55-62. | 1.5 | 26 |
| 2009 | An analysis of the changes in aromaticity and planarity along the reaction path of the simplest Diels-Alder reaction. Exploring the validity of different indicators of aromaticity. Computational and Theoretical Chemistry, 2005, 727, 165-171. | 1.5 | 59 |
| 2010 | Structure and fragmentation of glycine, alanine, serine and cysteine radical cations. A theoretical study. Computational and Theoretical Chemistry, 2005, 727, 191-197. | 1.5 | 63 |
| 2011 | DFT study of the fixation of CO by SPS-based pincer Rh(I) and Ir(I) complexes: Regioselectivity and reactivity. Computational and Theoretical Chemistry, 2005, 724, 73-79. | 1.5 | 11 |
| 2012 | A theoretical study on Cu(II)-chelating properties of curcumin and its implications for curcumin as a multipotent agent to combat Alzheimer's disease. Computational and Theoretical Chemistry, 2005, 757, 199-202. | 1.5 | 43 |
| 2013 | Theoretical studies of oxygen atom transfer from flavin to electron-rich substrates. Computational and Theoretical Chemistry, 2005, 757, 175-181. | 1.5 | 8 |
| 2014 | Molecular structure and vibrational spectra of lepidine and 2-chlorolepidine by density functional theory and ab initio Hartree-Fock Calculations. Computational and Theoretical Chemistry, 2005, 730, 59-67. | 1.5 | 19 |
| 2015 | Molecular geometry, electronic structure and optical properties study of meridional tris(8-hydroxyquinolinato)gallium(III) with ab initio and DFT methods. Computational and Theoretical Chemistry, 2005, 755, 19-30. | 1.5 | 17 |
| 2016 | Theoretical studies on neutral hydrolysis of N-benzyl 3-oxo- β -sultam. Computational and Theoretical Chemistry, 2005, 757, 61-68. | 1.5 | 1 |
| 2017 | Density functional theory study of W_n ($n=2-4$) clusters. Computational and Theoretical Chemistry, 2005, 757, 113-118. | 1.5 | 27 |
| 2018 | Dependence of metathesis activity of Mo-methylidene sites on their location on (100) β -Al ₂ O ₃ a theoretical study. Catalysis Today, 2005, 101, 163-173. | 2.2 | 33 |
| 2019 | Molecular structures of oxovanadium(IV) complexes with maltol and kojic acid: a quantum mechanical study. Inorganic Chemistry Communication, 2005, 8, 76-78. | 1.8 | 14 |
| 2020 | DFT investigations of models related to the active site of [NiFe] and [Fe] hydrogenases. Coordination Chemistry Reviews, 2005, 249, 1620-1640. | 9.5 | 123 |
| 2021 | Linear response at the 4-component relativistic density-functional level: application to the frequency-dependent dipole polarizability of Hg, AuH and PtH ₂ . Chemical Physics, 2005, 311, 187-201. | 0.9 | 71 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2022 | Electronic structures and band gaps of chains and sheets based on phenylacetylene units. Chemical Physics, 2005, 312, 289-297. | 0.9 | 43 |
| 2023 | DFT benchmark study for the oxidative addition of CH ₄ to Pd. Performance of various density functionals. Chemical Physics, 2005, 313, 261-270. | 0.9 | 94 |
| 2024 | Current-voltage curves for molecular junctions: Metal basis set vs. cluster size. Chemical Physics, 2005, 315, 293-296. | 0.9 | 4 |
| 2025 | A DFT study on the deprotonation antioxidant mechanistic step of ortho-substituted phenolic cation radicals. Chemical Physics, 2005, 316, 195-204. | 0.9 | 54 |
| 2026 | Electrostatic properties of polyethylene LB films on metal electrodes. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2005, 257-258, 287-290. | 2.3 | 4 |
| 2027 | Quickstep: Fast and accurate density functional calculations using a mixed Gaussian and plane waves approach. Computer Physics Communications, 2005, 167, 103-128. | 3.0 | 4,200 |
| 2028 | The effect of different density functional methods on basis set parameters. Chemical Physics Letters, 2005, 402, 510-513. | 1.2 | 30 |
| 2029 | Bond-based corrections to semi-empirical and ab initio electronic structure calculations. Chemical Physics Letters, 2005, 402, 524-528. | 1.2 | 12 |
| 2030 | Mass scaling for vibrational frequencies from ab initio calculations. Chemical Physics Letters, 2005, 403, 275-279. | 1.2 | 5 |
| 2031 | Structure and electron detachment energies of Si^{17+} . overflow= scroll xmlns:xocs= http://www.elsevier.com/xml/xocs/dtd xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tbl="http://www.elsevier.com/xml/common/table/dtd" xmlns:tbl_struct="http://www.elsevier.com/xml/common/table-struct/dtd" xmlns:td="http://www.elsevier.com/xml/ja/dtd" style="font-size: 10pt; font-family: serif; font-style: normal; font-weight: normal; text-align: left; vertical-align: top; white-space: normal; width: 100%; border-collapse: collapse;"> | 1.2 | 13 |
| 2032 | A theoretical study on the strength of two-center three-electron bond in (CH ₃) ₂ S-OH and H ₂ S-OH adducts. Chemical Physics Letters, 2005, 408, 216-220. | 1.2 | 14 |
| 2033 | Linear regression correction to first principle theoretical calculations - Improved descriptors and enlarged training set. Chemical Physics Letters, 2005, 409, 315-321. | 1.2 | 9 |
| 2034 | Time-dependent density functional theory for polycyclic aromatic hydrocarbon anions: What is the best approach. Chemical Physics Letters, 2005, 409, 235-239. | 1.2 | 10 |
| 2035 | Neural network correction for heats of formation with a larger experimental training set and new descriptors. Chemical Physics Letters, 2005, 410, 125-130. | 1.2 | 34 |
| 2036 | Ionization of carbon disulfide/ozone mixtures in atmospheric gases. Chemical Physics Letters, 2005, 410, 377-383. | 1.2 | 6 |
| 2037 | A theoretical measurement of the quantum transport through an optical molecular switch. Chemical Physics Letters, 2005, 412, 55-59. | 1.2 | 66 |
| 2038 | First principles calculations of thermodynamics for semiconductor alloys. Chemical Physics Letters, 2005, 412, 92-96. | 1.2 | 0 |
| 2039 | Ultrafast vibrational energy transfer from O-H stretching modes of liquid water. Chemical Physics Letters, 2005, 413, 176-181. | 1.2 | 9 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2040 | Is there a satisfactory description of the molecular structure of Roesky's ketone?. <i>Chemical Physics Letters</i> , 2005, 413, 440-444. | 1.2 | 11 |
| 2041 | Non-enzymatic oxidation of NADH by quinones. <i>Chemical Physics Letters</i> , 2005, 414, 243-247. | 1.2 | 13 |
| 2042 | Electron detachment energies of Al ₄ P ⁺ and Ga ₄ P ⁺ . <i>Chemical Physics Letters</i> , 2005, 414, 341-345. | 1.2 | 4 |
| 2043 | Fragmentation of heme and hemin ⁺ with sequential loss of carboxymethyl groups: A DFT and mass-spectrometry study. <i>Chemical Physics Letters</i> , 2005, 415, 362-369. | 1.2 | 37 |
| 2044 | Computational evidence in favor of a protonated chromophore in the photoactivation of phytochrome. <i>Chemical Physics Letters</i> , 2005, 416, 83-88. | 1.2 | 22 |
| 2045 | A new multivalent cluster: synthesis, electrochemistry, solid state structure and computational studies on the iron-nickel mixed-metal nitride anions [Fe ₆ Ni ₆ N ₂ (CO) ₂₄] ⁿ⁻ (n=2-4). <i>Comptes Rendus Chimie</i> , 2005, 8, 1850-1855. | 0.2 | 11 |
| 2046 | Combined experimental and theoretical DFT study of molecular nanowires negative differential resistance and interaction with gold clusters. <i>European Physical Journal E</i> , 2005, 18, 201-206. | 0.7 | 21 |
| 2047 | Benchmark Databases for Nonbonded Interactions and Their Use To Test Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 415-432. | 2.3 | 832 |
| 2048 | Density Functional Studies of Actinyl Aquo Complexes Studied Using Small-Core Effective Core Potentials and a Scalar Four-Component Relativistic Method. <i>Journal of Physical Chemistry A</i> , 2005, 109, 10961-10974. | 1.1 | 218 |
| 2049 | A General Study of Aryloxo and Alkoxo Ligands in the Titanium-Catalyzed Intermolecular Hydroamination of Terminal Alkynes. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 5001-5012. | 1.2 | 78 |
| 2050 | B3LYP density functional study on spectroscopic properties of CuO ⁺ and CuS ⁺ . <i>International Journal of Quantum Chemistry</i> , 2005, 105, 43-47. | 1.0 | 6 |
| 2051 | Photoreaction of Skin-sensitizing Trimethyl Psoralen with Lipid Membrane Models. <i>Photochemistry and Photobiology</i> , 2005, 81, 1153. | 1.3 | 7 |
| 2052 | Adsorption and Vibrational Spectroscopy of CO on Mordenite: Ab initio Density-Functional Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 7345-7357. | 1.2 | 32 |
| 2053 | Assessment of Gaussian-3 and density-functional theories on the G3/05 test set of experimental energies. <i>Journal of Chemical Physics</i> , 2005, 123, 124107. | 1.2 | 320 |
| 2054 | Local Aromaticity of [n]Acenes, [n]Phenacenes, and [n]Helicenes (n = 1-9). <i>Journal of Organic Chemistry</i> , 2005, 70, 2509-2521. | 1.7 | 195 |
| 2055 | Multidisciplinary Physicochemical Analysis of Oligothiophenes End-Capped by Nitriles: Electrochemistry, UV-Vis-Near-IR, IR, and Raman Spectroscopies and Quantum Chemistry. <i>Journal of Physical Chemistry B</i> , 2005, 109, 10115-10125. | 1.2 | 40 |
| 2056 | Supramolecular Chemistry of Halogens: Complementary Features of Inorganic (M ^X) and Organic (C ^X) Halogens Applied to M ^X -A _n -X ⁻ C Halogen Bond Formation. <i>Journal of the American Chemical Society</i> , 2005, 127, 5979-5989. | 6.6 | 365 |
| 2057 | Evaluation of a new copper(II)-curcumin complex as superoxide dismutase mimic and its free radical reactions. <i>Free Radical Biology and Medicine</i> , 2005, 39, 811-822. | 1.3 | 208 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2058 | Vibrational computations beyond the harmonic approximation: Performances of the B3LYP density functional for semirigid molecules. <i>Journal of Computational Chemistry</i> , 2005, 26, 384-388. | 1.5 | 179 |
| 2059 | Interaction of sodium and potassium ions with sandwiched cytosine-, guanine-, thymine-, and uracil-base tetrads. <i>Journal of Computational Chemistry</i> , 2005, 26, 352-364. | 1.5 | 34 |
| 2060 | Electronic structure study of the initiation routes of the dimethyl sulfide oxidation by OH. <i>Journal of Computational Chemistry</i> , 2005, 26, 569-583. | 1.5 | 27 |
| 2061 | Oxidative addition of the ethane C-C bond to Pd. An ab initio benchmark and DFT validation study. <i>Journal of Computational Chemistry</i> , 2005, 26, 1006-1020. | 1.5 | 69 |
| 2062 | First-principle studies of intermolecular and intramolecular catalysis of protonated cocaine. <i>Journal of Computational Chemistry</i> , 2005, 26, 980-986. | 1.5 | 50 |
| 2063 | Benchmarking approximate density functional theory. I.s/d excitation energies in 3d transition metal cations. <i>Journal of Computational Chemistry</i> , 2005, 26, 1505-1518. | 1.5 | 57 |
| 2064 | Effect of the axial cysteine ligand on the electronic structure and reactivity of high-valent iron(IV) oxo-porphyrins (Compound I): A theoretical study. <i>Journal of Computational Chemistry</i> , 2005, 26, 1600-1611. | 1.5 | 15 |
| 2065 | Solution, Structural and Catalytic Studies of Neutral MCl ₂ (M = Pd, Pt) Complexes of the N/E Mixed-Donor Ligands 2-(RECH ₂)C ₅ H ₄ N (RE = MeS, PhS, MeSe). <i>European Journal of Inorganic Chemistry</i> , 2005, 2005, 1048-1055. | 1.0 | 26 |
| 2066 | Trigonal-Prismatic vs. Octahedral Geometry for MnII Complexes with Innocent Didentate Ligands: A Subtle Difference as Shown by XRD and DFT on [Mn(acac) ₂ (bpy)]. <i>European Journal of Inorganic Chemistry</i> , 2005, 2005, 2255-2261. | 1.0 | 47 |
| 2067 | Influence of the Conformation of Salen Complexes on the Stereochemistry of the Asymmetric Epoxidation of Olefins. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 2566-2574. | 1.2 | 59 |
| 2068 | Entropy of Activation for Reactions in the Condensed Phase: A Theoretical Study of the S _N 2 Alkylation of Amines. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 3342-3347. | 1.2 | 1 |
| 2069 | Bis(trimethylsilyl)diazene revisited. Density functional theory (DFT) calculations of nitrogen NMR parameters of some azo-compounds. <i>Heteroatom Chemistry</i> , 2005, 16, 84-91. | 0.4 | 7 |
| 2070 | Conformational Analysis and CD Calculations of Methyl-Substituted 13-Tridecano-13-lactones. <i>Helvetica Chimica Acta</i> , 2005, 88, 194-209. | 1.0 | 11 |
| 2071 | Evidence for Interchange Ligand-Exchange Processes on Solvated Beryllium Cations. <i>Helvetica Chimica Acta</i> , 2005, 88, 911-922. | 1.0 | 45 |
| 2072 | Determination of the Atropisomeric Stability and Solution Conformation of Asymmetrically Substituted Biphenyls by Means of Vibrational Circular Dichroism (VCD). <i>Helvetica Chimica Acta</i> , 2005, 88, 2302-2314. | 1.0 | 7 |
| 2073 | Through versus Cross Electron Delocalization in Polytriacetylene Oligomers: A Computational Analysis. <i>ChemPhysChem</i> , 2005, 6, 511-519. | 1.0 | 16 |
| 2074 | Generalized Hybrid-Orbital Method for Combining Density Functional Theory with Molecular Mechanicals. <i>ChemPhysChem</i> , 2005, 6, 1853-1865. | 1.0 | 67 |
| 2075 | Experimental and Computational Studies of the Phenyl Radical Reaction with Propyne. <i>ChemPhysChem</i> , 2005, 6, 2075-2085. | 1.0 | 24 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2076 | NMR Spectroscopy Investigation of the Cooperative Nature of the Internal Rotational Motions in Acetophenone. <i>ChemPhysChem</i> , 2005, 6, 2086-2098. | 1.0 | 13 |
| 2077 | Aromaticity Analysis of Lithium Cation/ π Complexes of Aromatic Systems. <i>ChemPhysChem</i> , 2005, 6, 2552-2561. | 1.0 | 46 |
| 2078 | Experimental Detection of Theoretically Predicted N ₂ CO. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 462-465. | 7.2 | 31 |
| 2079 | Proton Sandwiches: Nonclassical Carbocations with Tetracoordinate Protons. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 2719-2723. | 7.2 | 45 |
| 2080 | Polyazide Chemistry: The First Binary Group 6 Azides, Mo(N ₃) ₆ , W(N ₃) ₆ , [Mo(N ₃) ₇] ⁻ , and [W(N ₃) ₇] ⁻ , and the [NW(N ₃) ₄] ⁻ and [NMo(N ₃) ₄] ⁻ Ions. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 1860-1865. | 7.2 | 87 |
| 2081 | Phenoxy Radicals Hydrogen-Bonded to Imidazolium: Analogues of Tyrosyl D. of Photosystem II: High-Field EPR and DFT Studies. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 5314-5317. | 7.2 | 73 |
| 2082 | Transition-State Effects of Ionic Liquids in Substitution Reactions of PtII Complexes. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 6033-6038. | 7.2 | 49 |
| 2088 | A statistical/collisional approach to rates of bimolecular reactions at low pressure. <i>International Journal of Chemical Kinetics</i> , 2005, 37, 233-242. | 1.0 | 2 |
| 2089 | Gas-phase tautomers of protonated 1-methylcytosine. Preparation, energetics, and dissociation mechanisms. <i>Journal of Mass Spectrometry</i> , 2005, 40, 1417-1428. | 0.7 | 25 |
| 2090 | High-field EPR investigations of MnIII/MnIV and MnII/MnIII states of dimanganese catalase and related model systems. <i>Magnetic Resonance in Chemistry</i> , 2005, 43, S51-S64. | 1.1 | 45 |
| 2091 | A QM/MM Study of the Asymmetric Dihydroxylation of Terminal Aliphatic Alkenes with OsO ₄ ·(DHQD)2PYDZ: Enantioselectivity as a Function of Chain Length. <i>Chemistry - A European Journal</i> , 2005, 11, 1017-1029. | 1.7 | 24 |
| 2092 | C ₅ H ₄ BR ₂ Bending in Ferrocenylboranes: A Delocalized Through-Space Interaction Between Iron and Boron. <i>Chemistry - A European Journal</i> , 2005, 11, 584-603. | 1.7 | 131 |
| 2093 | Experimental and Computational Studies of Hydrogen Bonding and Proton Transfer to [Cp*Fe(dppe)H]. <i>Chemistry - A European Journal</i> , 2005, 11, 873-888. | 1.7 | 58 |
| 2094 | The Breakdown of the Minimum Polarizability Principle in Vibrational Motions as an Indicator of the Most Aromatic Center. <i>Chemistry - A European Journal</i> , 2005, 11, 6024-6031. | 1.7 | 15 |
| 2095 | Nitrogen Fixation under Mild Ambient Conditions: Part I—The Initial Dissociation/Association Step at Molybdenum Triamidoamine Complexes. <i>Chemistry - A European Journal</i> , 2005, 11, 7448-7460. | 1.7 | 71 |
| 2096 | Accurate partial atomic charges for high-energy molecules using class IV charge models with the MIDI! basis set. <i>Theoretical Chemistry Accounts</i> , 2005, 113, 133-151. | 0.5 | 34 |
| 2097 | Geometric and electronic similarities between transition structures for electrocyclizations and sigmatropic hydrogen shifts. <i>Theoretical Chemistry Accounts</i> , 2005, 113, 205-211. | 0.5 | 6 |
| 2098 | Analysis of spin states, spin barriers, and trans-effects involved in the coordination and stabilization of dinitrogen by biomimetic iron complexes. <i>Theoretical Chemistry Accounts</i> , 2005, 114, 76-83. | 0.5 | 7 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2099 | Multipole electrostatic model for MNDO-like techniques with minimal valence spd-basis sets. <i>Theoretical Chemistry Accounts</i> , 2005, 114, 159-168. | 0.5 | 16 |
| 2100 | Gas phase UV and IR absorption spectra of CF ₃ CH ₂ CH ₂ OH and F(CF ₂ CF ₂) _x CH ₂ CH ₂ OH (x=2, 3, 4). <i>Journal of Fluorine Chemistry</i> , 2005, 126, 1288-1296. | 0.9 | 19 |
| 2101 | Structural motifs of DNA complexes in the gas phase. <i>International Journal of Mass Spectrometry</i> , 2005, 240, 183-193. | 0.7 | 101 |
| 2102 | Ammonia activation by iron: state-specific reactions of Fe+(6D, 4F) with ND ₃ and the reaction of FeNH+ with D ₂ . <i>International Journal of Mass Spectrometry</i> , 2005, 241, 243-260. | 0.7 | 24 |
| 2103 | Dissociation reactions of diatomic silver cations with small alkenes: experiment and theory. <i>International Journal of Mass Spectrometry</i> , 2005, 241, 99-108. | 0.7 | 19 |
| 2104 | Loss of water and hydrogen atom from the n-propanol molecular cation: A theoretical study. <i>International Journal of Mass Spectrometry</i> , 2005, 245, 53-60. | 0.7 | 6 |
| 2105 | How useful are vibrational frequencies of isotopomeric O ₂ fragments for assessing local symmetry? Some simple systems and the vexing case of a galactose oxidase model. <i>Journal of Biological Inorganic Chemistry</i> , 2005, 10, 778-789. | 1.1 | 26 |
| 2106 | Dimanganese catalase's spectroscopic parameters from broken-symmetry density functional theory of the superoxidized Mn(III)/Mn(IV) state. <i>Journal of Biological Inorganic Chemistry</i> , 2005, 10, 231-238. | 1.1 | 61 |
| 2107 | Regression formulae for ab initio and density functional calculated chemical shifts. <i>Journal of Molecular Modeling</i> , 2005, 11, 175-185. | 0.8 | 70 |
| 2108 | The structure and stability of B ₃₆ N ₃₆ cages: a computational study. <i>Journal of Molecular Modeling</i> , 2005, 12, 1-8. | 0.8 | 32 |
| 2109 | Electron delocalization in mixed-valence butadienediyl-bridged diruthenium complexes. <i>Journal of Solid State Electrochemistry</i> , 2005, 9, 738-749. | 1.2 | 36 |
| 2110 | Molecular quantum similarity using conceptual DFT descriptors. <i>Journal of Chemical Sciences</i> , 2005, 117, 425-435. | 0.7 | 29 |
| 2111 | Basis set effects on the energy and hardness profiles of the hydrogen fluoride dimer. <i>Journal of Chemical Sciences</i> , 2005, 117, 549-554. | 0.7 | 4 |
| 2112 | Regioselectivity in the [2 + 2] cyclo-addition reaction of triplet carbonyl compounds to substituted alkenes (Paterno-BÁchi reaction): A spin-polarized conceptual DFT approach. <i>Journal of Chemical Sciences</i> , 2005, 117, 561-571. | 0.7 | 20 |
| 2113 | Indirect Nuclear ⁷⁷ Se/ ⁷⁷ Se Spin-Spin Coupling Constants. Application of Density Functional Theory (DFT) Calculations. <i>Structural Chemistry</i> , 2005, 16, 67-71. | 1.0 | 10 |
| 2114 | A protein backbone γ and δ angle dependence of $2J_{N(i),C(i-1)}$: The new NMR experiment and quantum chemical calculations. <i>Journal of Biomolecular NMR</i> , 2005, 31, 87-95. | 1.6 | 10 |
| 2115 | Calculations of IR-spectra of metastable bond isomers of ruthenium nitrosocomplexes [Ru(NO)Cl ₅] ²⁻ [Ru(NO)(CN) ₅] ²⁻ by DFT method. <i>Journal of Structural Chemistry</i> , 2005, 46, 752-755. | 0.3 | 0 |
| 2116 | A DFT Study of Acetylenic Alkali Metal Thiolates. <i>Russian Journal of General Chemistry</i> , 2005, 75, 1142-1146. | 0.3 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2117 | NMR Studies of the Phosphazene/Phosphazane Rearrangement. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 85-89. | 0.6 | 3 |
| 2118 | Trichloropalladate(II) Complexes with Pyridine Ligands - Molecular Structure and Conformational Analysis of [K(18C6)][PdCl3(py)]. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 1456-1462. | 0.6 | 6 |
| 2119 | Organoplatinum Complexes of the N,N-Diisopropyl-diazabutadiene Ligand: A Structural and Spectroscopic Study. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 2669-2676. | 0.6 | 3 |
| 2120 | Theoretical prediction of the contact distance dependence of the electron transfer reactivity of the ClO/ClO [•] coupling system. International Journal of Quantum Chemistry, 2005, 101, 305-319. | 1.0 | 1 |
| 2121 | Energy analysis of the chemical bond in group IV and V complexes: A density functional theory study. International Journal of Quantum Chemistry, 2005, 101, 869-877. | 1.0 | 26 |
| 2122 | Density functional calculations of ¹⁹ F and ²³⁵ U NMR chemical shifts in uranium (VI) chloride fluorides UF ₆ n Cl n : Influence of the relativistic approximation and role of the exchange-correlation functional. International Journal of Quantum Chemistry, 2005, 101, 372-380. | 1.0 | 31 |
| 2123 | Ab initio and DFT investigation of the structures and properties of chloromethyl and chlorofluoromethyl peroxy radicals. International Journal of Quantum Chemistry, 2005, 102, 178-188. | 1.0 | 5 |
| 2124 | Ab initio and DFT modeling of stereoselective deamination of aziridines by nitrosyl chloride. International Journal of Quantum Chemistry, 2005, 102, 139-146. | 1.0 | 9 |
| 2125 | Ab initio EPR study of S [•] and Se [•] defects in alkali halides. International Journal of Quantum Chemistry, 2005, 102, 409-414. | 1.0 | 4 |
| 2126 | B3LYP, BLYP and PBE DFT band structures of the nucleotide base stacks. International Journal of Quantum Chemistry, 2005, 102, 422-426. | 1.0 | 18 |
| 2127 | Moments of the electron momentum density: Requirements for ab initio and density functional theory calculations. International Journal of Quantum Chemistry, 2005, 102, 673-683. | 1.0 | 33 |
| 2128 | Density functional study of the heme moiety of cytochrome c. International Journal of Quantum Chemistry, 2005, 102, 1002-1009. | 1.0 | 8 |
| 2129 | Localized hybrid exchange-correlation potentials for Kohn-Sham DFT calculations of NMR and EPR parameters. International Journal of Quantum Chemistry, 2005, 104, 261-271. | 1.0 | 30 |
| 2130 | Spectroscopic and DFT studies of donor-acceptor molecules containing phenylquinoline and phenothiazine moieties in various redox states. International Journal of Quantum Chemistry, 2005, 104, 635-644. | 1.0 | 7 |
| 2131 | Density functional theory study of the relative energies and structures of the chair, twist, and boat conformations of stannacyclohexane, 1-methylstannacyclohexane, and 1,1-dimethylstannacyclohexane. International Journal of Quantum Chemistry, 2005, 105, 416-428. | 1.0 | 5 |
| 2132 | Ab initio quantum chemical studies of fullerene molecules with substitutes C ₅₉ X [X = 3/4 Si, Ge, Sn], C ₅₉ X [•] [X = 3/4 B, Al, Ga, In], and C ₅₉ X [X = 3/4 N, P, As, Sb]. International Journal of Quantum Chemistry, 2005, 105, 429-436. | 1.0 | 37 |
| 2133 | Discrimination between diastereoisomeric dipeptides by IR-UV double resonance spectroscopy and ab initio calculations. International Journal of Quantum Chemistry, 2005, 105, 437-445. | 1.0 | 43 |
| 2134 | Relative energies, stereoelectronic interactions and conformational interconversions in silathiacyclohexanes. Journal of Physical Organic Chemistry, 2005, 18, 35-48. | 0.9 | 15 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2135 | Assessment of Clar's aromatic π -sextet rule by means of PDI, NICS and HOMA indicators of local aromaticity. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 785-791. | 0.9 | 147 |
| 2136 | Synthesis and conformational analysis of chiral ureas incorporating N-1-phenylethyl groups. Manifestation of allylic 1,3-strain. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 792-799. | 0.9 | 13 |
| 2137 | Vinyl or isopropenyl substituents as experimental and theoretical probes for diamagnetic anisotropies of aromatic hydrocarbons. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 800-817. | 0.9 | 5 |
| 2138 | Investigations of cluster ions formed between cesium cations and benzoic, salicylic and phthalic acids by electrospray mass spectrometry and density-functional theory calculations. Toward a modeling of the interaction of Cs ⁺ with humic substances. <i>Rapid Communications in Mass Spectrometry</i> , 2005, 19, 568-573. | 0.7 | 16 |
| 2139 | Pyridine N-oxide and pyridine-d 5 N-oxide: an electrospray/tandem mass spectrometric study carried out at high mass resolution. <i>Rapid Communications in Mass Spectrometry</i> , 2005, 19, 984-1004. | 0.7 | 6 |
| 2140 | The formation of neutral CCCO ₂ H and HCCCO ₂ molecules from anionic precursors in the gas phase: a joint experimental and theoretical study. <i>Rapid Communications in Mass Spectrometry</i> , 2005, 19, 3705-3712. | 0.7 | 3 |
| 2141 | Performance of binary-encounter-Bethe (BEB) theory for electron-impact ionization cross sections of molecules containing heavy elements ($Z > 10$). <i>Surface and Interface Analysis</i> , 2005, 37, 973-977. | 0.8 | 20 |
| 2142 | An exceptional P-H phosphonite: Biphenyl-2,2'-bis(fenyl)chlorophosphite and derived ligands (BIFOPs) in enantioselective copper-catalyzed 1,4-additions. <i>Beilstein Journal of Organic Chemistry</i> , 2005, 1, 6. | 1.3 | 17 |
| 2144 | Acetylene Cyclotrimerization by Early Second-Row Transition Metals in the Gas Phase. A Theoretical Study. <i>Inorganic Chemistry</i> , 2005, 44, 9807-9816. | 1.9 | 36 |
| 2145 | Variations in the Peak Position of the 6.2 μ m Interstellar Emission Feature: A Tracer of N in the Interstellar Polycyclic Aromatic Hydrocarbon Population. <i>Astrophysical Journal</i> , 2005, 632, 316-332. | 1.6 | 242 |
| 2146 | First-principles calculations of anharmonic vibrational spectroscopy of large molecules. , 2005, , 165-194. | | 42 |
| 2147 | Electronic structure. , 2005, , 483-505. | | 6 |
| 2148 | The optical gap of small Ge nanocrystals. <i>Journal of Physics: Conference Series</i> , 2005, 10, 97-100. | 0.3 | 10 |
| 2149 | Accurate and efficient treatment of two-electron contributions in quasirelativistic high-order Douglas-Kroll density-functional calculations. <i>Journal of Chemical Physics</i> , 2005, 123, 204113. | 1.2 | 91 |
| 2150 | Calculation of spin-densities within the context of density functional theory. The crucial role of the correlation functional. <i>Journal of Chemical Physics</i> , 2005, 123, 124101. | 1.2 | 37 |
| 2151 | Efficient methods for finding transition states in chemical reactions: Comparison of improved dimer method and partitioned rational function optimization method. <i>Journal of Chemical Physics</i> , 2005, 123, 224101. | 1.2 | 662 |
| 2152 | Ab initio multireference configuration-interaction theoretical study on the low-lying spin states in binuclear transition-metal complex: Magnetic exchange of [(NH ₃) ₅ Cr(¹ / ₄ -OH)Cr(NH ₃) ₅] ⁵⁺ and [Cl ₃ FeOFeCl ₃] ²⁻ . <i>Journal of Chemical Physics</i> , 2005, 122, 204310. | 1.2 | 15 |
| 2153 | Clusters of glycolic acid with three to six water molecules. <i>Journal of Chemical Physics</i> , 2005, 122, 074313. | 1.2 | 14 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2154 | CS ₂ O ⁺ and CS ₂ O in the gas phase: An experimental and computational study. <i>Journal of Chemical Physics</i> , 2005, 123, 164307. | 1.2 | 1 |
| 2155 | Binding at molecule/gold transport interfaces. V. Comparison of different metals and molecular bridges. <i>Journal of Chemical Physics</i> , 2005, 123, 234704. | 1.2 | 18 |
| 2156 | Cooperative versus dispersion effects: What is more important in an associated liquid such as water?. <i>Journal of Chemical Physics</i> , 2005, 123, 204116. | 1.2 | 62 |
| 2157 | Perturbational calculations of parity-violating effects in nuclear-magnetic-resonance parameters. <i>Journal of Chemical Physics</i> , 2005, 123, 054501. | 1.2 | 35 |
| 2158 | Orbital- and state-dependent functionals in density-functional theory. <i>Journal of Chemical Physics</i> , 2005, 123, 062203. | 1.2 | 125 |
| 2159 | Rotational barriers of a nitrophenylene ethynylene trimer. <i>Physical Review B</i> , 2005, 71, . | 1.1 | 5 |
| 2160 | Cubic response functions in time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2005, 122, 054107. | 1.2 | 71 |
| 2161 | Conformational Effects in Inner-Shell Photoelectron Spectroscopy of Ethanol. <i>Physical Review Letters</i> , 2005, 95, 103002. | 2.9 | 35 |
| 2162 | Theoretical study of the electronic spectroscopy of CO adsorbed on Pt(111). <i>Journal of Chemical Physics</i> , 2005, 122, 184706. | 1.2 | 19 |
| 2163 | Influence of the long-range exchange effect on dynamic polarizability. <i>Molecular Physics</i> , 2005, 103, 2183-2189. | 0.8 | 44 |
| 2164 | Torsional potential of 4,4'-bipyridine: Ab initio analysis of dispersion and vibrational effects. <i>Journal of Chemical Physics</i> , 2005, 123, 134309. | 1.2 | 37 |
| 2165 | High-pressure phases of FeTiO ₃ from first principles. <i>Physical Review B</i> , 2005, 72, . | 1.1 | 38 |
| 2166 | Linear scaling computation of the Fock matrix. VII. Periodic density functional theory at the Γ point. <i>Journal of Chemical Physics</i> , 2005, 122, 134102. | 1.2 | 11 |
| 2167 | An extended hybrid density functional (X3LYP) with improved descriptions of nonbond interactions and thermodynamic properties of molecular systems. <i>Journal of Chemical Physics</i> , 2005, 122, 014105. | 1.2 | 204 |
| 2168 | The structure and spin-states of some Fe(III) mimics of nitrile hydratase, studied by DFT and ONIOM(DFT:PM3) calculations. <i>Molecular Physics</i> , 2005, 103, 905-923. | 0.8 | 12 |
| 2169 | Quantum-Chemical Studies of Molecular Reactivity in Nanoporous Materials. , 2004, , 191-245. | | 4 |
| 2170 | Positively charged carbon vacancy in three inequivalent lattice sites of 6H- α -SiC: Combined EPR and density functional theory study. <i>Physical Review B</i> , 2005, 71, . | 1.1 | 26 |
| 2171 | Benchmark correlation energies for small molecules. <i>Molecular Physics</i> , 2005, 103, 763-766. | 0.8 | 48 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 2172 | Comparative analysis of local spin definitions. <i>Journal of Chemical Physics</i> , 2005, 122, 034102. | 1.2 | 87 |
| 2173 | THEORETICAL STUDY ON THE MECHANISM OF THE REACTION OF Ni(d10 1S) + H2 + CO2 → NiCO + H2O. <i>Journal of Theoretical and Computational Chemistry</i> , 2005, 04, 449-459. | 1.8 | 1 |
| 2174 | Acid-Base and Electronic Structure-Dependent Properties of Hoechst 33342. <i>Journal of Biomolecular Structure and Dynamics</i> , 2005, 23, 29-36. | 2.0 | 13 |
| 2175 | A Computational Study of Mixed Aggregates of Chloromethylithium with Lithium Dialkylamides. <i>Journal of Organic Chemistry</i> , 2005, 70, 8298-8302. | 1.7 | 9 |
| 2176 | Computational Characterization of the Role of the Base in the Suzuki-Miyaura Cross-Coupling Reaction. <i>Journal of the American Chemical Society</i> , 2005, 127, 9298-9307. | 6.6 | 317 |
| 2177 | SM6: A Density Functional Theory Continuum Solvation Model for Calculating Aqueous Solvation Free Energies of Neutrals, Ions, and Solute-Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1133-1152. | 2.3 | 414 |
| 2178 | Progress in the development of exchange-correlation functionals. , 2005, , 669-724. | | 108 |
| 2179 | Energetic Aspects of Cyclic Pi-Electron Delocalization: Evaluation of the Methods of Estimating Aromatic Stabilization Energies. <i>Chemical Reviews</i> , 2005, 105, 3773-3811. | 23.0 | 559 |
| 2180 | Interrelation between H-Bond and Pi-Electron Delocalization. <i>Chemical Reviews</i> , 2005, 105, 3513-3560. | 23.0 | 622 |
| 2181 | The Direct Detection of an Aryl Azide Excited State: An Ultrafast Study of the Photochemistry of para- and ortho-Biphenyl Azide. <i>Journal of the American Chemical Society</i> , 2005, 127, 13764-13765. | 6.6 | 44 |
| 2182 | An assessment of a simple hardness kernel approximation for the calculation of the global hardness in a series of Lewis acids and bases. <i>Computational and Theoretical Chemistry</i> , 2005, 727, 139-148. | 1.5 | 31 |
| 2183 | Application of the Palladium(0)-Catalyzed Ullmann Cross-Coupling Reaction in a Total Synthesis of (±)-Aspidospermidine and thus Representing an Approach to the Lower Hemisphere of the Binary Indole-Indoline Alkaloid Vinblastine. <i>Australian Journal of Chemistry</i> , 2005, 58, 722. | 0.5 | 40 |
| 2184 | Adsorption States of Dialkyl Ditelluride Autooxidized Monolayers on Au(111). <i>Langmuir</i> , 2005, 21, 3344-3353. | 1.6 | 22 |
| 2185 | Accurate ab Initio Binding Energies of Alkaline Earth Metal Clusters. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11927-11932. | 1.1 | 36 |
| 2186 | Steric Effects in Metathesis and Reduction Reactions of Phosphinimines with Catechol- and Pinacolboranes. <i>Inorganic Chemistry</i> , 2005, 44, 4301-4308. | 1.9 | 31 |
| 2187 | Magnitude of Zero-Point Vibrational Corrections to Optical Rotation in Rigid Organic Molecules: A Time-Dependent Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8617-8623. | 1.1 | 104 |
| 2188 | Density functional calculations of molecular parity-violating effects within the zeroth-order regular approximation. <i>Journal of Chemical Physics</i> , 2005, 122, 134316. | 1.2 | 43 |
| 2189 | Scaled DFT Force Constants and Vibrational Spectrum of Cyclopropylamine. <i>Spectroscopy Letters</i> , 2005, 38, 505-519. | 0.5 | 8 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2190 | Modulation of the electronic structure and the Ni-Fe distance in heterobimetallic models for the active site in [NiFe]hydrogenase. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 18280-18285. | 3.3 | 158 |
| 2191 | A comparison of density-functional-theory and coupled-cluster frequency-dependent polarizabilities and hyperpolarizabilities. Molecular Physics, 2005, 103, 439-450. | 0.8 | 74 |
| 2192 | A molecular dynamics study of the hydroxyl radical in solution applying self-interaction-corrected density functional methods. Physical Chemistry Chemical Physics, 2005, 7, 1363. | 1.3 | 159 |
| 2193 | One-electron oxidation of [CCOCC]â€“ TM in the gas phase forms stable and decomposing forms of CCCCCO. Organic and Biomolecular Chemistry, 2005, 3, 2646. | 1.5 | 2 |
| 2194 | Experimental and Theoretical Study of the Vibrational Spectra of Free 12-Crown-4. Journal of Physical Chemistry A, 2005, 109, 4505-4511. | 1.1 | 22 |
| 2195 | Investigation of a Putative Möbius Aromatic Hydrocarbon. The Effect of Benzannelation on Möbius [4n]Annulene Aromaticity. Journal of the American Chemical Society, 2005, 127, 2425-2432. | 6.6 | 100 |
| 2196 | Coordination properties of glycyglycine to Cu ⁺ , Ni ⁺ and Co ⁺ . Influence of metal cation electronic configuration. New Journal of Chemistry, 2005, 29, 1585. | 1.4 | 32 |
| 2197 | Effects of solvent on the relative stability of mono and di-aluminium aryloxide complexes of bipyridines: anomalous behavior of [(tBu)2Al(OPh)]2(1/4-4,4-bipy). Dalton Transactions, 2005, , 1722-1726. | 1.6 | 2 |
| 2198 | Multiresolution quantum chemistry in multiwavelet bases: time-dependent density functional theory with asymptotically corrected potentials in local density and generalized gradient approximations. Molecular Physics, 2005, 103, 413-424. | 0.8 | 109 |
| 2199 | Improved Density Functionals for Water. Journal of Physical Chemistry B, 2005, 109, 15677-15683. | 1.2 | 105 |
| 2200 | DFT-calculation of the structural isomers of (1-methyl-4-phenyl-1-azabuta-1,3-diene)tetracarbonyliron(0) and (4-phenyl-1-oxabuta-1,3-diene)tetracarbonyliron(0). Dalton Transactions, 2005, , 2933. | 1.6 | 3 |
| 2201 | Competing elimination and substitution reactions of simple acyclic disulfides. Organic and Biomolecular Chemistry, 2005, 3, 2095. | 1.5 | 18 |
| 2202 | Influence of the terminal ligands on the redox properties of the {Pt2(μ-S)2} core in [Pt2(Ph2X(CH2)2XPh2)2(μ-S)2](X = P or As) complexes and on their reactivity towards metal centres, protic acids and organic electrophiles. Dalton Transactions, 2005, , 2742. | 1.6 | 28 |
| 2203 | Neutral cumulene oxide CCCCCO is accessible by one-electron oxidation of [CCCCO]â€“ TM in the gas phase. Organic and Biomolecular Chemistry, 2005, 3, 901-910. | 1.5 | 5 |
| 2204 | Gas phase protonation of trifluoromethyl sulfur pentafluoride. Physical Chemistry Chemical Physics, 2005, 7, 1181. | 1.3 | 10 |
| 2205 | Activation of CH4by gas-phase Ni ⁺ and the thermochemistry of Niâ€“ligand complexes. Physical Chemistry Chemical Physics, 2005, 7, 1054-1064. | 1.3 | 46 |
| 2206 | Accelerated, energy-conserving Bornâ€“Oppenheimer molecular dynamics via Fock matrix extrapolation. Physical Chemistry Chemical Physics, 2005, 7, 3269. | 1.3 | 96 |
| 2207 | Câ€“H Activations at Iridium(I) Square-Planar Complexes Promoted by a Fifth Ligand. Journal of the American Chemical Society, 2005, 127, 18074-18084. | 6.6 | 23 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2208 | Multi-coefficient extrapolated density functional theory for thermochemistry and thermochemical kinetics. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 43. | 1.3 | 393 |
| 2209 | Synthesis of the Pivalamidate-Bridged Pentanuclear Platinum(II,III) Linear Complexes with Pt- μ_2 -Pt Interactions. <i>Inorganic Chemistry</i> , 2005, 44, 8552-8560. | 1.9 | 32 |
| 2210 | Structural Analysis of Metal Interactions with the Dinucleotide Duplex, dCG-dCG, Using Ion Mobility Mass Spectrometry. <i>Journal of Physical Chemistry B</i> , 2005, 109, 4808-4810. | 1.2 | 21 |
| 2211 | Reactions of Methane with Titanium Atoms: CH_3TiH , CH_2TiH_2 , Agostic Bonding, and $(\text{CH}_3)_2\text{TiH}_2$. <i>Inorganic Chemistry</i> , 2005, 44, 4834-4842. | 1.9 | 57 |
| 2212 | Photogenerated N-Methyl-N-1-naphthylnitrenium Ion: Laser Flash Photolysis, Trapping Rates, and Product Study. <i>Journal of Organic Chemistry</i> , 2005, 70, 3127-3132. | 1.7 | 15 |
| 2213 | Infrared Spectra of CH_3CrH , CH_3WH , CH_2WH_2 , and CH_2WH_3 Formed by Activation of CH_4 with Cr and W Atoms. <i>Inorganic Chemistry</i> , 2005, 44, 7634-7643. | 1.9 | 44 |
| 2214 | Theoretical Investigation of Uranyl Dihydroxide: Oxo Ligand Exchange, Water Catalysis, and Vibrational Spectra. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8579-8586. | 1.1 | 35 |
| 2215 | Reaction of Tungsten η^5 -Acetylide Complexes $[(\eta^5\text{-C}_5\text{H}_5)(\text{NO})(\text{CO})\text{W}(\text{C}\equiv\text{R})\text{Li}]$ with Iminium Ions. <i>Organometallics</i> , 2005, 24, 977-989. | 1.1 | 16 |
| 2216 | Chemical Behavior of the Biradicaloid $(\text{HO})_2\text{ONO}$ Singlet States of Peroxynitrous Acid. The Oxidation of Hydrocarbons, Sulfides, and Selenides. <i>Journal of the American Chemical Society</i> , 2005, 127, 3140-3155. | 6.6 | 26 |
| 2217 | Photoelectron Spectroscopy of Doubly and Singly Charged Group VIB Dimetalate Anions: $\text{M}_2\text{O}_7^{2-}$, MMO_7^- , and M_2O_7^- (M, $\text{M} = \text{Cr, Mo, W}$). <i>Journal of Physical Chemistry A</i> , 2005, 109, 10512-10520. | 1.1 | 73 |
| 2218 | Metathesis Activity and Properties of $\text{Mo}=\text{C}(\text{alkylidene})$ Sites Differently Located on Silica. A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 20794-20804. | 1.2 | 48 |
| 2219 | A Theoretical Study of the Formation of the Parent Phosphinine $\text{C}_5\text{H}_5\text{P}$ from the Flash Vacuum Thermolysis of Diallylvinylphosphine. <i>Journal of Organic Chemistry</i> , 2005, 70, 4637-4642. | 1.7 | 10 |
| 2220 | B3LYP and MP2 Calculations of the Enthalpies of Hydrogen-Bonded Complexes of Methanol with Neutral Bases and Anions: Comparison with Experimental Data. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11907-11913. | 1.1 | 75 |
| 2221 | Effect of Dehydration on Sulfate Coordination and Speciation at the $\text{Fe}(\text{Hydr})\text{oxide}/\text{Water}$ Interface: A Molecular Orbital/Density Functional Theory and Fourier Transform Infrared Spectroscopic Investigation. <i>Langmuir</i> , 2005, 21, 11071-11078. | 1.6 | 64 |
| 2222 | Multicenter Bond Indices As a New Means for the Quantitative Characterization of Homoaromaticity. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6606-6609. | 1.1 | 50 |
| 2223 | Adiabatic Electron Affinities of the Polyhydrated Adenine-Thymine Base Pair: A Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3971-3979. | 1.1 | 43 |
| 2224 | Chiral Zirconium Catalysts Using Multidentate BINOL Derivatives for Catalytic Enantioselective Mannich-Type Reactions; Ligand Optimization and Approaches to Elucidation of the Catalyst Structure. <i>Journal of the American Chemical Society</i> , 2005, 127, 15528-15535. | 6.6 | 54 |
| 2225 | Computational Studies of the Thermal Fragmentation of P-Arylphosphiranes: Have Arylphosphinidenes Been Generated by This Method?. <i>Journal of the American Chemical Society</i> , 2005, 127, 9886-9894. | 6.6 | 20 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2226 | Synthesis and X-ray Crystal Structure of a Cationic Homoleptic (SPS) ₂ Rh(III) Complex and EPR Study of Its Reduction Process. <i>Inorganic Chemistry</i> , 2005, 44, 1147-1152. | 1.9 | 15 |
| 2227 | How Well Can Density Functional Methods Describe Hydrogen Bonds to π Acceptors?. <i>Journal of Physical Chemistry B</i> , 2005, 109, 19046-19051. | 1.2 | 169 |
| 2228 | The Asymmetric Schrock Olefin Metathesis Catalyst. A Computational Study. <i>Organometallics</i> , 2005, 24, 3200-3206. | 1.1 | 46 |
| 2229 | G3(MP2) Study of the C ₃ H ₆ O+ π Isomers Fragmented from 1,4-Dioxane+ π . <i>Journal of Physical Chemistry A</i> , 2005, 109, 7296-7308. | 1.1 | 1 |
| 2230 | Mapping the Triplet Potential Energy Surface of 1-Methyl-8-nitronaphthalene. <i>Journal of Organic Chemistry</i> , 2005, 70, 6074-6084. | 1.7 | 1 |
| 2231 | Structure, Bonding, and Solvation of Lithium Vinylcarbenoids. <i>Journal of Organic Chemistry</i> , 2005, 70, 2294-2298. | 1.7 | 24 |
| 2232 | π -CH π -N Substitutedmer-Gaq ₃ andmer-Alq ₃ Derivatives: An Effective Approach for the Tuning of Emitting Color. <i>Journal of Physical Chemistry B</i> , 2005, 109, 17762-17767. | 1.2 | 47 |
| 2233 | Solvation Properties of N-Substituted Cis and Trans Amides Are Not Identical: Significant Enthalpy and Entropy Changes Are Revealed by the Use of Variable Temperature ¹ H NMR in Aqueous and Chloroform Solutions and ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11878-11884. | 1.1 | 17 |
| 2234 | Uranyl Complexation in Fluorinated Acids (HF, HBF ₄ , HPF ₆ , HTf ₂ N): A Combined Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , 2005, 44, 852-861. | 1.9 | 39 |
| 2235 | Ligand-to-Diimine/Metal-to-Diimine Charge-Transfer Excited States of [Re(NCS)(CO) ₃ (π -diimine)] (π -diimine) Tj ETQq1 1 0.784314 rgBT <i>Physical Chemistry A</i> , 2005, 109, 5016-5025. | 1.1 | 68 |
| 2236 | Donor-Stabilized Silyl Cations. 9. Two Dissociation Patterns of Hexacoordinate Silicon Complexes: A Model Nucleophilic Substitution at Pentacoordinate Silicon. <i>Organometallics</i> , 2005, 24, 2913-2920. | 1.1 | 41 |
| 2237 | Conformations and Tautomers of 5a,6-Anhydrotetracycline. <i>Journal of Physical Chemistry B</i> , 2005, 109, 4279-4284. | 1.2 | 9 |
| 2238 | Synthesis of Chiral Self-Assembling Rhombs and Their Characterization in Solution, in the Gas Phase, and at the Liquid-Solid Interface. <i>Journal of the American Chemical Society</i> , 2005, 127, 17672-17685. | 6.6 | 61 |
| 2239 | Uncovering Transport Properties of 4,4'-Bipyridine/Gold Molecular Nanobridges. <i>Journal of Physical Chemistry B</i> , 2005, 109, 10052-10060. | 1.2 | 35 |
| 2240 | Fe π -N π -O Structure and Bonding in Six-Coordinate {FeNO} ₆ Porphyrinates Containing Imidazole: Implications for Reactivity of Coordinated NO. <i>Inorganic Chemistry</i> , 2005, 44, 1367-1380. | 1.9 | 36 |
| 2241 | An ab Initio Study of SN ₂ Reactivity at C ₆ in Hexopyranose Derivatives. I. Influence of Dipole-Dipole Interactions in the Transition Structure. <i>Journal of Physical Chemistry A</i> , 2005, 109, 213-217. | 1.1 | 1 |
| 2242 | Real space optical gap calculations in oxygenated Si nanocrystals. <i>Journal of Physics: Conference Series</i> , 2005, 10, 69-72. | 0.3 | 4 |
| 2243 | Bonding Pattern Continuum from Covalent to Dative Carbon-Silicon Bonds for Substituted Silenes: A Theoretical Study. <i>Organometallics</i> , 2005, 24, 3746-3752. | 1.1 | 6 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2244 | Experimental and Theoretical Studies of Carbodiphosphorane σ -CX ₂ Adducts with Unusual Bonding Situations: A Preparation, Crystal Structures, and Bonding Analyses of S ₂ CC(PPh ₃) ₂ , O ₂ CC(PPh ₃) ₂ , and [(CO) ₄ MS ₂ CC(PPh ₃) ₂] (M = Cr, Mo, W). <i>Inorganic Chemistry</i> , 2005, 44, 1263-1274. | 1.9 | 90 |
| 2245 | Experimental and Theoretical Studies of the C ₂ F ₄ + O Reaction: A Nonadiabatic Reaction Mechanism. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9786-9794. | 1.1 | 7 |
| 2246 | Estimation, Computation, and Experimental Correction of Molecular Zero-Point Vibrational Energies. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6779-6789. | 1.1 | 47 |
| 2247 | 19-Electron Intermediates and Cage-Effects in the Photochemical Disproportionation of [CpW(CO) ₃] ₂ with Lewis Bases. <i>Journal of the American Chemical Society</i> , 2005, 127, 12555-12565. | 6.6 | 26 |
| 2248 | Infrared Spectra of the CH ₃ σ -CrF, CH ₂ WHF, and CH σ -WH ₂ F Molecules: A Reversible Photochemical Interconversion by H-Hydrogen Transfer. <i>Organometallics</i> , 2005, 24, 5678-5685. | 1.1 | 26 |
| 2249 | Remote Substituent Effects upon the Rearrangements of Housane Cation Radicals. <i>Journal of Organic Chemistry</i> , 2005, 70, 4598-4608. | 1.7 | 17 |
| 2250 | All-Electron Hybrid Density Functional Calculations on UFn and UCl _n (n = 1-6). <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 612-616. | 2.3 | 36 |
| 2251 | Theoretical Mechanistic Study of Rhodium(I) Phosphine-Catalyzed H/D Exchange Processes in Aqueous Solutions. <i>Organometallics</i> , 2005, 24, 3059-3065. | 1.1 | 49 |
| 2252 | Optical Properties and Delocalization of Excess Negative Charges on Oligo(Phenylenevinylene)s: A Quantum Chemical Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5644-5652. | 1.2 | 21 |
| 2253 | Databases for Transition Element Bonding: A Metal-Metal Bond Energies and Bond Lengths and Their Use To Test Hybrid, Hybrid Meta, and Meta Density Functionals and Generalized Gradient Approximations. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4388-4403. | 1.1 | 209 |
| 2254 | Tailoring Transition Metal Complexes for Nonlinear Optics Applications. 2. A Theoretical Investigation of the Second-Order Nonlinear Optical Properties of M(CO) ₅ L Complexes (M = Cr, W; L = Py, PyCHO.) <i>Journal of Physical Chemistry B</i> , 2005, 109, 20737-20745. | 1.2 | 16 |
| 2255 | Synthesis and Characterization of Three Novel Perfluoro-oligothiophenes Ranging in Length from the Trimer to the Pentamer. <i>Journal of Physical Chemistry B</i> , 2005, 109, 20737-20745. | 1.2 | 16 |
| 2256 | Influence of Cu ⁺ on the RS σ -NO Bond Dissociation Energy of S-Nitrosothiols. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1334-1336. | 1.2 | 34 |
| 2257 | Comparative Study of Surface Cycloadditions of Ethylene and 2-Butene on the Si(100)-2 \times 1 Surface. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5067-5072. | 1.2 | 23 |
| 2258 | New Selective Haloform-type Reaction Yielding 3-Hydroxy-2,2-difluoroacids: A Theoretical Study of the Mechanism. <i>Journal of the American Chemical Society</i> , 2005, 127, 2620-2627. | 6.6 | 12 |
| 2259 | Geometrical and Electronic Structures of Dinuclear Complex Ions $\{(\eta^4\text{-bpym})[\text{Cu}(\text{EAr}_3)_2]_2\}^{2+}$ with Intramolecular σ -Organic Sandwich Formation (E = P or As; Ar = Aryl; bpym = 2,2'-Bipyrimidine). <i>Inorganic Chemistry</i> , 2005, 44, 4637-4643. | 1.9 | 23 |
| 2260 | PCM Study of the Solvent and Substituent Effects on the Conformers, Intramolecular Hydrogen Bonds and Bond Dissociation Enthalpies of 2-Substituted Phenols. <i>Journal of Physical Chemistry A</i> , 2005, 109, 366-377. | 1.1 | 42 |
| 2261 | Theoretical Investigation of the Reactivity of Copper Atoms with OCS: A Comparison with CS ₂ and CO ₂ . <i>Journal of Physical Chemistry A</i> , 2005, 109, 7932-7937. | 1.1 | 25 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2262 | Switching End-on to Side-on $\text{C}\pi\text{-N}$ Coordination: A Computational Approach. <i>Organometallics</i> , 2005, 24, 6037-6042. | 1.1 | 15 |
| 2263 | Quantum Chemical and Master Equation Simulations of the Oxidation and Isomerization of Vinyloxy Radicals. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2514-2524. | 1.1 | 43 |
| 2264 | Reactions of Platinum(II)-diketones with 2-Aminopyridines: Synthesis and Characterization of Aminocarbene Complexes of Platinum(II). <i>Organometallics</i> , 2005, 24, 533-538. | 1.1 | 18 |
| 2265 | A Combined Quantum and Molecular Mechanical Study of the O_2 Reductive Cleavage in the Catalytic Cycle of Multicopper Oxidases. <i>Inorganic Chemistry</i> , 2005, 44, 5612-5628. | 1.9 | 79 |
| 2266 | Modeling Multiple Species of Nicotine and Deschloroepibatidine Interacting with AChR Nicotinic Acetylcholine Receptor: From Microscopic Binding to Phenomenological Binding Affinity. <i>Journal of the American Chemical Society</i> , 2005, 127, 14401-14414. | 6.6 | 46 |
| 2267 | Calculation of Electron Detachment Energies for Water Cluster Anions: An Appraisal of Electronic Structure Methods, with Application to $(\text{H}_2\text{O})_{20}^-$ and $(\text{H}_2\text{O})_{24}^-$. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5217-5229. | 1.1 | 139 |
| 2268 | Second Half-Reaction of Nitric Oxide Synthase: Computational Insights into the Initial Step and Key Proposed Intermediate. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23706-23714. | 1.2 | 28 |
| 2269 | Ultrafast Infrared Mechanistic Studies of the Interaction of 1-Hexyne with Group 6 Hexacarbonyl Complexes. <i>Organometallics</i> , 2005, 24, 1852-1859. | 1.1 | 28 |
| 2270 | Gold as Hydrogen. An Experimental and Theoretical Study of the Structures and Bonding in Disilicon Gold Clusters Si_2Au_n and Si_2Au_n ($n=2$ and 4) and Comparisons to Si_2H_2 and Si_2H_4 . <i>Journal of Physical Chemistry A</i> , 2005, 109, 4366-4374. | 1.1 | 104 |
| 2271 | Extraordinary Cluster Formation and Intramolecular Ligand-Ligand Interactions in Cyanoacetylene Mediated by Mg^+ : Implications for the Atmospheric Chemistry of Titan and for Circumstellar Chemistry. <i>Journal of the American Chemical Society</i> , 2005, 127, 13070-13078. | 6.6 | 12 |
| 2272 | Electronic and Structural Evolution and Chemical Bonding in Tungsten Oxide Clusters: W_2O_n and W_2O_n ($n=1-6$). <i>Journal of Physical Chemistry A</i> , 2005, 109, 6019-6030. | 1.1 | 67 |
| 2273 | Performance of Molecular Orbital Methods and Density Functional Theory in the Computation of Geometries and Energies of Metal Aqua Ions. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1510-1527. | 1.2 | 102 |
| 2274 | An Intramolecularly Base-Stabilized Diphosphagermylene and Two Unusual Germanium(II) Ate Complexes: A Structural, NMR, and DFT Study. <i>Organometallics</i> , 2005, 24, 2157-2167. | 1.1 | 35 |
| 2275 | Theoretical Studies of Alkyl Radicals in the NaY and HY Zeolites. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7242-7250. | 1.1 | 14 |
| 2276 | Thermal Decomposition of Ethylene Oxide: Potential Energy Surface, Master Equation Analysis, and Detailed Kinetic Modeling. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8016-8027. | 1.1 | 38 |
| 2277 | Thermodynamic and Strain Effects in the Competition between 5-Exo-dig and 6-Endo-dig Cyclizations of Vinyl and Aryl Radicals. <i>Journal of the American Chemical Society</i> , 2005, 127, 12583-12594. | 6.6 | 88 |
| 2278 | Photodegradation of Substituted Stilbene Compounds: What Colors Aging Paper Yellow?. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5677-5682. | 1.1 | 10 |
| 2279 | Intrinsic Carbon-Carbon Bond Reactivity at the Manganese Center of Oxalate Decarboxylase from <i>Density Functional Theory</i> . <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 994-1007. | 2.3 | 11 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2280 | Infrared and Computational Investigation of Vanadium-Substituted Keggin [PVnW12-nO40](n+3)-Polyoxometallic Anions. <i>Journal of Physical Chemistry B</i> , 2005, 109, 8928-8934. | 1.2 | 20 |
| 2281 | Experimental and Theoretical Study of Stabilization of Delocalized Forms of Semibullvalenes and Barbaralanes by Dipolar and Polarizable Solvents. Observation of a Delocalized Structure that Is Lower in Free Energy than the Localized Form. <i>Journal of Organic Chemistry</i> , 2005, 70, 3437-3449. | 1.7 | 37 |
| 2282 | Theoretical Investigations of Uranyl ^{VI} Ligand Bonding: Four- and Five-Coordinate Uranyl Cyanide, Isocyanide, Carbonyl, and Hydroxide Complexes. <i>Inorganic Chemistry</i> , 2005, 44, 2255-2262. | 1.9 | 103 |
| 2283 | Design of Density Functionals That Are Broadly Accurate for Thermochemistry, Thermochemical Kinetics, and Nonbonded Interactions. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5656-5667. | 1.1 | 1,451 |
| 2284 | Multidimensional Description of the Aromaticity in Planar Five-Membered NSNS Ring Systems. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4847-4851. | 1.1 | 12 |
| 2285 | Performance of Nonrelativistic and Quasi-Relativistic Hybrid DFT for the Prediction of Electric and Magnetic Hyperfine Parameters in ⁵⁷ Fe Mössbauer Spectra. <i>Inorganic Chemistry</i> , 2005, 44, 2245-2254. | 1.9 | 214 |
| 2286 | Cytosine Catalysis of Nitrosative Guanine Deamination and Interstrand Cross-Link Formation. <i>Journal of the American Chemical Society</i> , 2005, 127, 7346-7358. | 6.6 | 26 |
| 2287 | Which Do Endohedral Ti ₂ C ₈₀ Metallofullerenes Prefer Energetically: Ti ₂ @C ₈₀ or Ti ₂ C ₂ @C ₇₈ ? A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 20251-20255. | 1.2 | 78 |
| 2288 | Spin-Polarized Conceptual Density Functional Theory Study of the Regioselectivity in the [2+2] Photocycloaddition of Enones to Substituted Alkenes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6335-6343. | 1.1 | 44 |
| 2289 | Adenine Radicals in the Gas Phase: An Experimental and Computational Study of Hydrogen Atom Adducts to Adenine. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8121-8132. | 1.1 | 33 |
| 2290 | N,O-Dilithio-2-(N-methylamino)ethanol: An Intramolecular Mixed Aggregate. <i>Journal of Organic Chemistry</i> , 2005, 70, 101-104. | 1.7 | 8 |
| 2291 | 5-Endo-Dig Radical Cyclizations: The Poor Cousins of the Radical Cyclizations Family. <i>Journal of the American Chemical Society</i> , 2005, 127, 9534-9545. | 6.6 | 66 |
| 2292 | DFT Computational Study of the Mechanism of Allyl Chloride Carbonylation Catalyzed by Palladium Complexes. <i>Organometallics</i> , 2005, 24, 2086-2096. | 1.1 | 16 |
| 2293 | Search for Stratospheric Bromine Reservoir Species: Theoretical Study of the Photostability of Mono-, Tri-, and Pentacoordinated Bromine Compounds. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8133-8139. | 1.1 | 5 |
| 2294 | Acidity of a Cu-Bound Histidine in the Binuclear Center of Cytochrome c Oxidase. <i>Journal of Physical Chemistry B</i> , 2005, 109, 22629-22640. | 1.2 | 27 |
| 2295 | Insight into Enzymatic C-H Bond Formation from QM and QM/MM Calculations. <i>Journal of the American Chemical Society</i> , 2005, 127, 13643-13655. | 6.6 | 80 |
| 2296 | Marked Variations of Dissociation Energy and H-Bond Character of the Guanine-Cytosine Base Pair Induced by One-Electron Oxidation and Li ⁺ Cation Coupling. <i>Journal of Physical Chemistry B</i> , 2005, 109, 593-600. | 1.2 | 22 |
| 2297 | Binding Energy Curves from Nonempirical Density Functionals. I. Covalent Bonds in Closed-Shell and Radical Molecules. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11006-11014. | 1.1 | 57 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2298 | Oxidative Addition of the Fluoromethane C-F Bond to Pd. An ab Initio Benchmark and DFT Validation Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9685-9699. | 1.1 | 61 |
| 2299 | New Effective Core Method (Effective Core Potential and Valence Basis Set) for Al Clusters and Nanoparticles and Heteronuclear Al-Containing Molecules. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 41-53. | 2.3 | 21 |
| 2300 | Cycloaddition Isomerizations of Adsorbed 1,3-Cyclohexadiene on Si(100)-2 \times 1 Surface: First Neighbor Interactions. <i>Journal of the American Chemical Society</i> , 2005, 127, 8485-8491. | 6.6 | 17 |
| 2301 | Structure, Bonding, and Reactivity of the Organometallic 1,3,2,4-Dithiadiazole Complex CpCoS ₂ N ₂ . <i>Organometallics</i> , 2005, 24, 1004-1011. | 1.1 | 18 |
| 2302 | Influence of Resonance on the Acidity of Sulfides, Sulfoxides, Sulfones, and Their Group 16 Congeners. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4966-4972. | 1.1 | 18 |
| 2303 | Alternated Quinoid/Aromatic Units in Terthiophenes Building Blocks for Electroactive Narrow Band Gap Polymers. Extended Spectroscopic, Solid State, Electrochemical, and Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 16616-16627. | 1.2 | 48 |
| 2304 | Fourier Transform Raman and Density Functional Theory Studies on the Adsorption Behavior of p-Hydroxybenzoic Acid on Silver Nanoparticles. <i>Journal of Physical Chemistry B</i> , 2005, 109, 21865-21867. | 1.2 | 10 |
| 2305 | Modeling the Absorption Spectrum of Tryptophan in Proteins. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23061-23069. | 1.2 | 46 |
| 2306 | Cross-Linking between Thymine and Indolyl Radical: A Possible Mechanism for Cross-Linking of DNA and Tryptophan-Containing Peptides. <i>Bioconjugate Chemistry</i> , 2005, 16, 588-597. | 1.8 | 10 |
| 2307 | Effect of Packing and Tilt on the Rotational Barriers of an Amino, Nitro-Substituted Phenylene Ethynylene Trimer. <i>Journal of Physical Chemistry B</i> , 2005, 109, 9059-9065. | 1.2 | 5 |
| 2308 | Planar and Pyramidal Tetracoordinate Carbon in Organoboron Compounds. <i>Journal of Organic Chemistry</i> , 2005, 70, 6693-6704. | 1.7 | 56 |
| 2309 | Backbone and Side-Chain Cleavages in Electron Detachment Dissociation (EDD). <i>Journal of Physical Chemistry A</i> , 2005, 109, 11332-11337. | 1.1 | 60 |
| 2310 | Surface-Stabilized Amorphous Germanium Nanoparticles for Lithium-Storage Material. <i>Journal of Physical Chemistry B</i> , 2005, 109, 20719-20723. | 1.2 | 112 |
| 2311 | The electronic spectrum of protonated adenine: Theory and experiment. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3306. | 1.3 | 96 |
| 2312 | Benchmark Database of Barrier Heights for Heavy Atom Transfer, Nucleophilic Substitution, Association, and Unimolecular Reactions and Its Use to Test Theoretical Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2012-2018. | 1.1 | 736 |
| 2313 | Activation Energies of Pericyclic Reactions: A Performance of DFT, MP2, and CBS-QB3 Methods for the Prediction of Activation Barriers and Reaction Energetics of 1,3-Dipolar Cycloadditions, and Revised Activation Enthalpies for a Standard Set of Hydrocarbon Pericyclic Reactions. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9542-9553. | 1.1 | 233 |
| 2314 | π -Aromaticity and π -Antiaromaticity in Saturated Inorganic Rings. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3711-3716. | 1.1 | 60 |
| 2315 | Potential Energy Surfaces, Product Distributions and Thermal Rate Coefficients of the Reaction of O(3P) with C ₂ H ₄ (X1Ag): A Comprehensive Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7489-7499. | 1.1 | 91 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2316 | \hat{I}^2 -Lactam antibiotics are multipotent agents to combat neurological diseases. <i>Biochemical and Biophysical Research Communications</i> , 2005, 333, 661-663. | 1.0 | 40 |
| 2317 | Ab-initio structure, energy and stable Cr isotopes equilibrium fractionation of some geochemically relevant H-O-Cr-Cl complexes. <i>Geochimica Et Cosmochimica Acta</i> , 2005, 69, 851-874. | 1.6 | 19 |
| 2318 | Ab initio thermochemistry of some geochemically relevant molecules in the system Cr-O-H-Cl. <i>Geochimica Et Cosmochimica Acta</i> , 2005, 69, 3505-3518. | 1.6 | 5 |
| 2319 | First principle study of the adsorption of atomic hydrogen on cluster-model surfaces. <i>Synthetic Metals</i> , 2005, 152, 329-332. | 2.1 | 6 |
| 2320 | Modeling solvent effects on electron-spin-resonance hyperfine couplings by frozen-density embedding. <i>Journal of Chemical Physics</i> , 2005, 123, 114101. | 1.2 | 64 |
| 2321 | Photochemical Generation of Highly Destabilized Vinyl Cations: The Effects of \hat{I}^{\pm} - and \hat{I}^2 -Trifluoromethyl versus \hat{I}^{\pm} - and \hat{I}^2 -Methyl Substituents. <i>Journal of Organic Chemistry</i> , 2005, 70, 179-190. | 1.7 | 31 |
| 2322 | The Cationic Cascade Route to Longifolene. <i>Journal of Organic Chemistry</i> , 2005, 70, 5139-5143. | 1.7 | 16 |
| 2323 | Designing meaningful density functional theory calculations in materials science—a primer. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2005, 13, R1-R31. | 0.8 | 342 |
| 2324 | How well can new-generation density functional methods describe stacking interactions in biological systems?. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 2701. | 1.3 | 246 |
| 2325 | Structure and UV-Vis spectroscopy of the iron-sulfur dinuclear nitrosyl complexes $[\text{Fe}_2\text{S}_2(\text{NO})_4]^{2+}$ and $[\text{Fe}_2(\text{SR})_2(\text{NO})_4]$. <i>New Journal of Chemistry</i> , 2005, 29, 604. | 1.4 | 48 |
| 2326 | Evaluation of Functionals O3LYP, KMLYP, and MPW1K in Comparison to B3LYP for Selected Transition-Metal Compounds. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 848-855. | 2.3 | 54 |
| 2327 | Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions. <i>Journal of Chemical Physics</i> , 2005, 123, 161103. | 1.2 | 979 |
| 2328 | Where Is the Spin? Understanding Electronic Structure and g-Tensors for Ruthenium Complexes with Redox-Active Quinonoid Ligands. <i>Journal of the American Chemical Society</i> , 2005, 127, 11399-11413. | 6.6 | 164 |
| 2329 | The Final Catalytic Step of Cytochrome P450 Aromatase: A Density Functional Theory Study. <i>Journal of the American Chemical Society</i> , 2005, 127, 5224-5237. | 6.6 | 103 |
| 2330 | The Peculiar Trend of Cyclic Perfluoroalkane Electron Affinities with Increasing Ring Size. <i>Journal of the American Chemical Society</i> , 2005, 127, 15457-15469. | 6.6 | 29 |
| 2331 | Tautomers and electronic states of jet-cooled 2-aminopurine investigated by double resonance spectroscopy and theory. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3021. | 1.3 | 59 |
| 2332 | Electron-Impact Ionization Cross Sections of Molecules Containing Heavy Elements ($Z > 10$). <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1153-1161. | 2.3 | 16 |
| 2333 | Polarizable continuum model study of solvent effects on electronic circular dichroism parameters. <i>Journal of Chemical Physics</i> , 2005, 122, 024106. | 1.2 | 58 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2334 | Hydrogen-bonding interactions in acetic acid monohydrates and dihydrates by density-functional theory calculations. <i>Journal of Chemical Physics</i> , 2005, 123, 074325. | 1.2 | 34 |
| 2335 | MODELING VIBRATIONAL SPECTRA USING THE SELF-CONSISTENT CHARGE DENSITY-FUNCTIONAL TIGHT-BINDING METHOD II: INFRARED SPECTRA. <i>Journal of Theoretical and Computational Chemistry</i> , 2005, 04, 639-655. | 1.8 | 27 |
| 2336 | Interface Geometry and Molecular Junction Conductance: Geometric Fluctuation and Stochastic Switching. <i>Nano Letters</i> , 2005, 5, 1668-1675. | 4.5 | 236 |
| 2337 | Incisive Structure Spectroscopic Correlation in Oligothiophenes Functionalized with ($\hat{A}\pm$) Inductive/Mesomeric Fluorine Groups: A Joint Raman and DFT Study. <i>Journal of the American Chemical Society</i> , 2005, 127, 13364-13372. | 6.6 | 29 |
| 2338 | Nonradical Zinc Barbier Reaction for Diastereoselective Synthesis of Vicinal Amino Alcohols. <i>Journal of the American Chemical Society</i> , 2005, 127, 15756-15761. | 6.6 | 67 |
| 2339 | Determination of the Absolute Configuration of Threos-Hydrindacene Compounds by Vibrational Circular Dichroism. <i>Journal of Organic Chemistry</i> , 2005, 70, 9103-9114. | 1.7 | 47 |
| 2340 | Natural Energy Decomposition Analysis: Extension to Density Functional Methods and Analysis of Cooperative Effects in Water Clusters. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11936-11940. | 1.1 | 245 |
| 2341 | Mechanistic Aspects of Pyrite Oxidation in an Oxidizing Gaseous Environment: An In Situ HATR IR Isotope Study. <i>Environmental Science & Technology</i> , 2005, 39, 7576-7584. | 4.6 | 43 |
| 2342 | Adsorption of NH ₃ and H ₂ O in Acidic Chabazite. Comparison of ONIOM Approach with Periodic Calculations. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3539-3545. | 1.2 | 96 |
| 2343 | Synthesis and structural study of new highly lipophilic 1,4-dihydropyridines. <i>New Journal of Chemistry</i> , 2005, 29, 1567. | 1.4 | 17 |
| 2344 | Hypervalent ammonium radicals. Competitive N-C and N-H bond dissociations in methyl ammonium and ethyl ammonium. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 912-920. | 1.3 | 35 |
| 2345 | Gold behaves as hydrogen: Prediction on the existence of a new class of boron-containing radicals, AuBX (X=F,Cl,Br). <i>Journal of Chemical Physics</i> , 2005, 123, 241101. | 1.2 | 22 |
| 2346 | Mechanism of Formation of Organic Carbonates from Aliphatic Alcohols and Carbon Dioxide under Mild Conditions Promoted by Carbodiimides. DFT Calculation and Experimental Study. <i>Journal of Organic Chemistry</i> , 2005, 70, 6177-6186. | 1.7 | 90 |
| 2347 | Real-space post-Hartree-Fock correlation models. <i>Journal of Chemical Physics</i> , 2005, 122, 064101. | 1.2 | 231 |
| 2348 | Ab Initio and DFT Study of the ²⁹ Si NMR Chemical Shifts in RSi ₄ SiR. <i>Organometallics</i> , 2005, 24, 6319-6330. | 1.1 | 43 |
| 2349 | Growth of ZnO thin films: experiment and theory. <i>Journal of Materials Chemistry</i> , 2005, 15, 139-148. | 6.7 | 364 |
| 2350 | Density Functional Methods for Excited States: Equilibrium Structure and Electronic Spectra. <i>Theoretical and Computational Chemistry</i> , 2005, 16, 93-128. | 0.2 | 192 |
| 2351 | Stiffness and Raman Intensity: A Conceptual and Computational DFT Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6071-6076. | 1.1 | 21 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 2352 | Treatment of Substitution and Rearrangement Mechanisms of Transition Metal Complexes with Quantum Chemical Methods. <i>Chemical Reviews</i> , 2005, 105, 2003-2038. | 23.0 | 167 |
| 2353 | A new pathway for the rapid decay of electronically excited adenine. <i>Journal of Chemical Physics</i> , 2005, 122, 104314. | 1.2 | 217 |
| 2354 | Accurate Calculation of the Heats of Formation for Large Main Group Compounds with Spin-Component Scaled MP2 Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3067-3077. | 1.1 | 241 |
| 2355 | Structures and Properties of Self-Assembled Monolayers of Bistable [2]Rotaxanes on Au (111) Surfaces from Molecular Dynamics Simulations Validated with Experiment. <i>Journal of the American Chemical Society</i> , 2005, 127, 1563-1575. | 6.6 | 202 |
| 2356 | One-Dimensional BeH ₂ Polymers: Infrared Spectra and Theoretical Calculations. <i>Inorganic Chemistry</i> , 2005, 44, 610-614. | 1.9 | 32 |
| 2357 | Density-functional calculations of relativistic spin-orbit effects on nuclear magnetic shielding in paramagnetic molecules. <i>Journal of Chemical Physics</i> , 2005, 123, 174102. | 1.2 | 50 |
| 2358 | Density Functional Theory Study of Optical Transitions in Semiconducting Single-Walled Carbon Nanotubes. <i>Nano Letters</i> , 2005, 5, 1621-1624. | 4.5 | 92 |
| 2359 | The Reaction of Acetylene with Hydroxyl Radicals. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6045-6055. | 1.1 | 86 |
| 2360 | Infinite-Basis Calculations of Binding Energies for the Hydrogen Bonded and Stacked Tetramers of Formic Acid and Formamide and Their Use for Validation of Hybrid DFT and ab Initio Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6624-6627. | 1.1 | 89 |
| 2361 | Assessment of Density Functionals for Predicting One-Bond Carbon-13 Hydrogen NMR Spin-Spin Coupling Constants. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 541-545. | 2.3 | 66 |
| 2362 | Theoretical Study on the Reaction Mechanism of the Gas-Phase H ₂ /CO ₂ /Ni(3D) System. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6498-6502. | 1.1 | 13 |
| 2363 | Quantum Chemical and Master Equation Studies of the Methyl Vinyl Carbonyl Oxides Formed in Isoprene Ozonolysis. <i>Journal of Physical Chemistry A</i> , 2005, 109, 10710-10725. | 1.1 | 56 |
| 2364 | Semiempirical hybrid functional with improved performance in an extensive chemical assessment. <i>Journal of Chemical Physics</i> , 2005, 123, 121103. | 1.2 | 131 |
| 2365 | Ligand-Assisted Reduction of Osmium Tetroxide with Molecular Hydrogen via a [3+2] Mechanism. <i>Journal of the American Chemical Society</i> , 2005, 127, 3423-3432. | 6.6 | 37 |
| 2366 | A Computational Study of Oxiranyllithium. <i>Journal of Organic Chemistry</i> , 2005, 70, 7238-7242. | 1.7 | 14 |
| 2367 | Mesitylthio-Oligothiophenes in Various Redox States. Molecular and Electronic Views as Offered by Spectroscopy and Theory. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11275-11284. | 1.1 | 21 |
| 2368 | Mechanisms of Difluoroethylene Ozonolysis: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9284-9291. | 1.1 | 6 |
| 2369 | A Comparative Study of the Catalytic Mechanisms of the Zinc and Cadmium Containing Carbonic Anhydrase. <i>Journal of the American Chemical Society</i> , 2005, 127, 4242-4253. | 6.6 | 75 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2370 | Theoretical Study of the Highly Diastereoselective 1,3-Dipolar Cycloaddition of 1,4-Dihydropyridine-Containing Azomethine Ylides to [60]Fullerene (Prato's Reaction). <i>Journal of Organic Chemistry</i> , 2005, 70, 3256-3262. | 1.7 | 36 |
| 2371 | Structure and properties of ilmenite from first principles. <i>Physical Review B</i> , 2005, 71, . | 1.1 | 98 |
| 2372 | Conformational Study of the Structure of 12-crown-4 ⁺ Alkali Metal Cation Complexes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8041-8048. | 1.1 | 21 |
| 2373 | Density Functionals for Inorganometallic and Organometallic Chemistry. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11127-11143. | 1.1 | 447 |
| 2374 | Density Functional Energetics of α -Quartz for Calibration of SiO ₂ Interatomic Potentials. <i>Journal of Physical Chemistry B</i> , 2005, 109, 4168-4171. | 1.2 | 8 |
| 2375 | TDDFT Study of One- and Two-Photon Absorption Properties: π -Donor- π -Acceptor Chromophores. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1803-1814. | 1.2 | 101 |
| 2376 | Prescription for the design and selection of density functional approximations: More constraint satisfaction with fewer fits. <i>Journal of Chemical Physics</i> , 2005, 123, 062201. | 1.2 | 769 |
| 2377 | Interaction of Co ⁺ and Co ²⁺ with Glycine. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 224-230. | 1.1 | 42 |
| 2379 | Elucidation of the Thermochemical Properties of Triphenyl- or Tributyl-Substituted Si-, Ge-, and Sn-Centered Radicals by Means of Electrochemical Approaches and Computations. <i>Journal of the American Chemical Society</i> , 2005, 127, 2677-2685. | 6.6 | 22 |
| 2380 | Mechanism of Alkane C-H Bond Activation by Copper and Silver Homoscorpionate Complexes. <i>Organometallics</i> , 2006, 25, 5292-5300. | 1.1 | 84 |
| 2381 | Solid-State Modeling of the Terahertz Spectrum of the High Explosive HMX. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1951-1959. | 1.1 | 166 |
| 2382 | Proton-Transfer and H ₂ -Elimination Reactions of Main-Group Hydrides EH ₄ (E = B, Al, Ga) with Alcohols. <i>Inorganic Chemistry</i> , 2006, 45, 3086-3096. | 1.9 | 49 |
| 2383 | The performance of semilocal and hybrid density functionals in 3d transition-metal chemistry. <i>Journal of Chemical Physics</i> , 2006, 124, 044103. | 1.2 | 528 |
| 2384 | Biliverdine-Based Metalloradicals: π -Sterically Enhanced Noninnocence. <i>Inorganic Chemistry</i> , 2006, 45, 4914-4921. | 1.9 | 21 |
| 2385 | Dimers of and Tautomerism between 2-Pyrimidinethiol and 2(1H)-Pyrimidinethione: A Density Functional Theory (DFT) Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7904-7912. | 1.1 | 14 |
| 2386 | Single Crystals of β -O-Serine Phosphate X-Irradiated at Low Temperatures: EPR, ENDOR, EIE, and DFT Studies. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9585-9596. | 1.1 | 18 |
| 2387 | Cooperativity in ionic liquids. <i>Journal of Chemical Physics</i> , 2006, 124, 174506. | 1.2 | 153 |
| 2388 | Towards chemical accuracy for the thermodynamics of large molecules: new hybrid density functionals including non-local correlation effects. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 4398. | 1.3 | 538 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2389 | Molecular Dynamics Simulations of the Enzyme Cu, Zn Superoxide Dismutase. <i>Journal of Physical Chemistry B</i> , 2006, 110, 16754-16762. | 1.2 | 28 |
| 2390 | Metal-metal bonding in molecular actinide compounds: electronic structure of $[M_2X_8]^{2-}$ (M = U, Np). <i>Journal of Physical Chemistry B</i> , 2006, 110, 5476-5483. | 1.6 | 39 |
| 2391 | Density functional theory including dispersion corrections for intermolecular interactions in a large benchmark set of biologically relevant molecules. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 5287. | 1.3 | 446 |
| 2392 | Determination of the Absolute Configurations of Natural Products via Density Functional Theory Calculations of Optical Rotation, Electronic Circular Dichroism, and Vibrational Circular Dichroism: The Cytotoxic Sesquiterpene Natural Products Quadrone, Suberosenone, Suberosanone, and Suberosenol A Acetate. <i>Journal of Natural Products</i> , 2006, 69, 1055-1064. | 1.5 | 106 |
| 2393 | The Arginine Anomaly: Arginine Radicals Are Poor Hydrogen Atom Donors in Electron Transfer Induced Dissociations. <i>Journal of the American Chemical Society</i> , 2006, 128, 12520-12530. | 6.6 | 79 |
| 2394 | Ultrafast electron diffraction: Excited state structures and chemistries of aromatic carbonyls. <i>Journal of Chemical Physics</i> , 2006, 124, 174707. | 1.2 | 63 |
| 2395 | Theoretical Characterization of End-On and Side-On Peroxide Coordination in Ligated Cu_2O_2 Models. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11557-11568. | 1.1 | 80 |
| 2396 | Kinetics, Mechanism, and Computational Studies of Rhenium-Catalyzed Desulfurization Reactions of Thiiranes (Thioepoxides). <i>Inorganic Chemistry</i> , 2006, 45, 5351-5357. | 1.9 | 16 |
| 2397 | Experimental and Theoretical Investigations of IR Spectra and Electronic Structures of the $U(OH)_2$, $UO_2(OH)$, and $UO_2(OH)_2$ Molecules. <i>Inorganic Chemistry</i> , 2006, 45, 4157-4166. | 1.9 | 23 |
| 2398 | Intramolecular Interligand Charge Transfer in Hexacoordinate Silicon Complexes. <i>Organometallics</i> , 2006, 25, 2929-2933. | 1.1 | 29 |
| 2399 | Thermodynamic and Kinetic Studies on Reactions of Pt(II) Complexes with Biologically Relevant Nucleophiles. <i>Inorganic Chemistry</i> , 2006, 45, 2948-2959. | 1.9 | 136 |
| 2400 | Hydride Donor Abilities of Cationic Transition Metal Hydrides from DFT-PCM Calculations. <i>Organometallics</i> , 2006, 25, 820-825. | 1.1 | 31 |
| 2401 | Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Polycyclic Aromatic Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13624-13631. | 1.1 | 41 |
| 2402 | A new enantiomerization mechanism for tripodal penta-coordinate $ZnII(NTA)$ complexes. Theoretical clarification of the observed 1H NMR spectrum. <i>Dalton Transactions</i> , 2006, , 3392. | 1.6 | 19 |
| 2403 | Density Functional Theory Study of Tetrathiafulvalene and Thianthrene in Acetonitrile: Structure, Dynamics, and Redox Properties. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3614-3623. | 1.2 | 38 |
| 2404 | Influence of Coulomb-attenuation on exchange-correlation functional quality. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 4543-4549. | 1.3 | 127 |
| 2405 | Theoretical Studies of the Transition-State Structures and Free Energy Barriers for Base-Catalyzed Hydrolysis of Amides. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12644-12652. | 1.1 | 56 |
| 2406 | Exploration of the potential energy surface of C_4H_4 for rearrangement and decomposition reactions of vinylacetylene: A computational study. Part I. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 5304. | 1.3 | 53 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2407 | Mono- vs. bi-metallic assembly on a bulky bis(imino)terpyridine framework: a combined experimental and theoretical study. <i>Dalton Transactions</i> , 2006, , 2350-2361. | 1.6 | 29 |
| 2408 | Copper(II) Hexaaza Macrocyclic Binuclear Complexes Obtained from the Reaction of Their Copper(I) Derivates and Molecular Dioxygen. <i>Inorganic Chemistry</i> , 2006, 45, 3569-3581. | 1.9 | 61 |
| 2409 | Comparative assessment of density functional methods for 3d transition-metal chemistry. <i>Journal of Chemical Physics</i> , 2006, 124, 224105. | 1.2 | 180 |
| 2410 | Early Excited State Dynamics of 6-Styryl-Substituted Pyrylium Salts Exhibiting Dual Fluorescence. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9988-9994. | 1.1 | 27 |
| 2411 | Proteinâ€“cofactor interactions in bacterial reaction centers from <i>Rhodobacter sphaeroides</i> R-26: Effect of hydrogen bonding on the electronic and geometric structure of the primary quinone. A density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 5659-5670. | 1.3 | 41 |
| 2412 | Reaction of Ethylene with Hydroxyl Radicals: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6960-6970. | 1.1 | 156 |
| 2413 | Reaction of H ₂ with a Binuclear Zirconium Dinitrogen Complex âˆ’ Evaluation of Theoretical Models and Hybrid Approaches. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1298-1316. | 2.3 | 16 |
| 2414 | Ruthenium Tetraoxide Oxidations of Alkanes: DFT Calculations of Barrier Heights and Kinetic Isotope Effects. <i>Journal of Organic Chemistry</i> , 2006, 71, 1755-1760. | 1.7 | 38 |
| 2415 | Dielsâˆ’Alder Reactions of Cyclopentadiene and 9,10-Dimethylantracene with Cyanoalkenes: The Performance of Density Functional Theory and Hartreeâˆ’Fock Calculations for the Prediction of Substituent Effects. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1216-1224. | 1.1 | 67 |
| 2416 | SPOCK.CI: A multireference spin-orbit configuration interaction method for large molecules. <i>Journal of Chemical Physics</i> , 2006, 124, 124101. | 1.2 | 105 |
| 2417 | High accuracy calculations of the optical gap and absorption spectrum of oxygen contaminated Si nanocrystals. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 808-813. | 1.3 | 45 |
| 2418 | Nitrous Oxide Decomposition over Fe-ZSM-5 in the Presence of Nitric Oxide: A Comprehensive DFT Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17096-17114. | 1.2 | 77 |
| 2419 | pH-Dependent Electronic and Spectroscopic Properties of Pyridoxine (Vitamin B ₆). <i>Journal of Physical Chemistry B</i> , 2006, 110, 16774-16780. | 1.2 | 37 |
| 2420 | Mononuclear metavanadate catalyses gas phase oxidation of methanol to formaldehyde employing dioxygen as the terminal oxidant. <i>Chemical Communications</i> , 2006, , 4503. | 2.2 | 43 |
| 2421 | Structure of sodium bis(N-methyl-iminodiacetato)iron(III): trans-meridional N-coordination in the solid state and in solution. <i>Dalton Transactions</i> , 2006, , 5506. | 1.6 | 12 |
| 2422 | Theoretical study of the ground and excited states of 7-methyl guanine and 9-methyl guanine: comparison with experiment. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3059-3065. | 1.3 | 30 |
| 2423 | A combined Raman, DFT and MD study of the solvation dynamics and the adsorption process of pyridine in silver hydrosols. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 171-178. | 1.3 | 38 |
| 2424 | Lineshapes in carbon 1s photoelectron spectra of methanol clusters. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 2473-2482. | 1.3 | 23 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2425 | Structural, spectroscopic, and electrochemical behavior of trans-phenolato cobalt(iii) complexes of asymmetric NNâ€²O ligands as archetypes for metallomesogens. Dalton Transactions, 2006, , 2517-2525. | 1.6 | 55 |
| 2426 | Hydration effect on interaction mode between glutamic acid and Ca ²⁺ and its biochemical implication: a theoretical exploration. New Journal of Chemistry, 2006, 30, 890. | 1.4 | 2 |
| 2427 | Oxygen insertion in a carbonâ€“phosphorus bond of the phenylethynyl-di-(tert-butyl)-phosphine bridged dicobalt complex: exploring the nature of oxygen migration using DFT. Dalton Transactions, 2006, , 5454-5463. | 1.6 | 3 |
| 2428 | S3O and S3O ⁺ in the gas phase: ring and open-chain structures. Chemical Communications, 2006, , 4416. | 2.2 | 6 |
| 2429 | Density functional theory investigation of the geometric and electronic structures of [UO ₂ (H ₂ O) _m (OH) _n] ²⁺ (n + m = 5). Dalton Transactions, 2006, , 2403-2414. | 1.6 | 60 |
| 2430 | Reactivity of titanium dimer and molecular nitrogen in rare gas matrices. Vibrational and electronic spectra and structure of Ti ₂ N ₂ . Physical Chemistry Chemical Physics, 2006, 8, 2000-2011. | 1.3 | 26 |
| 2431 | Auolysis of Î±-C-deprotonated group 6 aminocarbene and thiocarbene complexes with Ph ₃ PAu ⁺ . Dalton Transactions, 2006, , 4580-4589. | 1.6 | 14 |
| 2432 | Degradation of Ionized OV(OCH ₃) ₃ in the Gas Phase. From the Neutral Compound All the Way down to the Quasi-terminal Fragments VO ⁺ and VOH ⁺ . Inorganic Chemistry, 2006, 45, 6235-6245. | 1.9 | 75 |
| 2433 | Quantum Chemical Calculations of Sulfate Adsorption at the Al- and Fe-(Hydr)oxide-H ₂ O Interface Estimation of Gibbs Free Energies. Environmental Science & Technology, 2006, 40, 7717-7724. | 4.6 | 58 |
| 2434 | Multireference Ab Initio Calculations on Reaction Intermediates of the Multicopper Oxidases. Inorganic Chemistry, 2006, 45, 11051-11059. | 1.9 | 42 |
| 2435 | Is the Hypothiocyanite Anion (OSCN ⁻) the Major Product in the Peroxidase Catalyzed Oxidation of the Thiocyanate Anion (SCN ⁻)? A Joint Experimental and Theoretical Study. Journal of Physical Chemistry A, 2006, 110, 4930-4936. | 1.1 | 13 |
| 2436 | Mechanistic Insights into the Reaction between VO ₂ ⁺ and Propene Based on a DFT Study. Organometallics, 2006, 25, 1643-1653. | 1.1 | 28 |
| 2437 | Radical Ions of Î±,Î±-Bis(diphenylamino)-capped Oligothiophenes: A Combined Spectroelectrochemical and Theoretical Study. Journal of Physical Chemistry B, 2006, 110, 8223-8231. | 1.2 | 46 |
| 2438 | Threshold Photoelectronâ“Photoion Coincidence Spectroscopy: Dissociation Dynamics and Thermochemistry of Ge(CH ₃) ₄ , Ge(CH ₃) ₃ Cl, and Ge(CH ₃) ₃ Br. Journal of Physical Chemistry A, 2006, 110, 5032-5037. | 1.1 | 11 |
| 2439 | Quantum-size effects in capped and uncapped carbon nanotubes. Annual Reports on the Progress of Chemistry Section C, 2006, 102, 71. | 4.4 | 16 |
| 2440 | Accuracy and limitations of second-order many-body perturbation theory for predicting vertical detachment energies of solvated-electron clusters. Physical Chemistry Chemical Physics, 2006, 8, 68-78. | 1.3 | 84 |
| 2441 | Structural, spectroscopic and magnetic properties of M[R ₂ P(E)NP(E)Râ€²] ₂ complexes, M = Co, Mn, E = S, Se and R, Râ€² = Ph or iPr. Covalency of Mâ€“S bonds from experimental data and theoretical calculations. Dalton Transactions, 2006, , 2301-2315. | 1.6 | 35 |
| 2442 | Role of defects in ferromagnetism in Zn _{1-x} Co _x O: A hybrid density-functional study. Physical Review B, 2006, 74, . | 1.1 | 190 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2443 | Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 364-382. | 2.3 | 3,329 |
| 2444 | Correlation between atomic rearrangement in defective fullerenes and migration behavior of encaged metal ions. <i>Physical Review B</i> , 2006, 73, . | 1.1 | 14 |
| 2445 | Aryl Transfer between Pd(II) Centers or Pd(IV) Intermediates in Pd-Catalyzed Domino Reactions. <i>Journal of the American Chemical Society</i> , 2006, 128, 5033-5040. | 6.6 | 177 |
| 2446 | A DFT Study of the Full Catalytic Cycle of the Suzuki-Miyaura Cross-Coupling on a Model System. <i>Organometallics</i> , 2006, 25, 3647-3658. | 1.1 | 348 |
| 2447 | Electron Delocalization and Aromaticity in Linear Polyacenes: Atoms in Molecules Multicenter Delocalization Index. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7642-7648. | 1.1 | 176 |
| 2448 | A Critical Analysis of the Cyclic and Open Alternatives of the Transmetalation Step in the Stille Cross-Coupling Reaction. <i>Journal of the American Chemical Society</i> , 2006, 128, 14571-14578. | 6.6 | 100 |
| 2449 | Extension of the Alkane Bridge in BisNHC-Palladium-Chloride Complexes. Synthesis, Structure, and Catalytic Activity. <i>Organometallics</i> , 2006, 25, 5409-5415. | 1.1 | 179 |
| 2450 | Structural and Electronic Characterization of the Complexes Obtained by the Interaction between Bare and Hydrated First-Row Transition-Metal Ions (Mn ²⁺ , Fe ²⁺ , Co ²⁺ , Ni ²⁺ , Cu ²⁺ , Zn ²⁺) and Glycine. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24666-24673. | 1.2 | 106 |
| 2451 | A Density Functional That Accounts for Medium-Range Correlation Energies in Organic Chemistry. <i>Organic Letters</i> , 2006, 8, 5753-5755. | 2.4 | 193 |
| 2452 | Dinuclear C,N,C Cyclometalated Platinum Derivatives with Bridging Delocalized Ligands. Fourfold Deprotonation of 6,6'-Diphenyl-2,2'-bipyridine, H ₄ L, Promoted by Pt(R) ₂ Fragments (R = Me, Ph). Crystal Structures of [Pt ₂ (L)(3,5-Me ₂ py) ₂] and {Pt ₂ (L)(dppe)} ₂ (dppe = 1,2-Bis(diphenylphosphino)ethane). X-ray Powder Diffraction of [Pt ₂ (L)(CO) ₂]. <i>Organometallics</i> , 2006, 25, 2253-2265. | 1.1 | 43 |
| 2453 | Comparative DFT Study of van der Waals Complexes: Rare-Gas Dimers, Alkaline-Earth Dimers, Zinc Dimer, and Zinc-Rare-Gas Dimers. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5121-5129. | 1.1 | 706 |
| 2454 | Two-component relativistic density-functional calculations of the dimers of the halogens from bromine through element 117 using effective core potential and all-electron methods. <i>Journal of Chemical Physics</i> , 2006, 124, 064305. | 1.2 | 70 |
| 2455 | Characterization and Surface Reactivity of Ferrihydrite Nanoparticles Assembled in Ferritin. <i>Langmuir</i> , 2006, 22, 9313-9321. | 1.6 | 53 |
| 2456 | Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides. <i>Physical Review B</i> , 2006, 74, . | 1.1 | 309 |
| 2457 | Binding of Gold Clusters with DNA Base Pairs: A Density Functional Study of Neutral and Anionic GC _n Aun and AT _n Aun (n = 4, 8) Complexes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7719-7727. | 1.1 | 70 |
| 2458 | 2-Phenylpyridine: To Twist or Not To Twist?. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1530-1537. | 2.3 | 11 |
| 2459 | Permeability of Psoralen Derivatives in Lipid Membranes. <i>Biophysical Journal</i> , 2006, 91, 2464-2474. | 0.2 | 27 |
| 2460 | Characterization of a Catalytic Ligand Bridging Metal Ions in Phosphodiesterases 4 and 5 by Molecular Dynamics Simulations and Hybrid Quantum Mechanical/Molecular Mechanical Calculations. <i>Biophysical Journal</i> , 2006, 91, 1858-1867. | 0.2 | 36 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2461 | Mechanism of Olefin Hydrosilylation Catalyzed by RuCl ₂ (CO) ₂ (PPh ₃) ₂ : A DFT Study. <i>Organometallics</i> , 2006, 25, 4504-4513. | 1.1 | 49 |
| 2462 | Regioselectivity in lithiation of 1-methylpyrazole: experimental, density functional theory and multinuclear NMR study. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 1261. | 1.5 | 13 |
| 2463 | Interplay between Intramolecular Resonance-Assisted Hydrogen Bonding and Aromaticity in o-Hydroxyaryl Aldehydes. <i>Journal of Organic Chemistry</i> , 2006, 71, 5241-5248. | 1.7 | 110 |
| 2464 | The formation of the stable radicals $\dot{\text{E}}^{\text{TM}}\text{CH}_2\text{CN}$, $\text{CH}_3\dot{\text{E}}^{\text{TM}}\text{CHCN}$ and $\dot{\text{E}}^{\text{TM}}\text{CH}_2\text{CH}_2\text{CN}$ from the anions CH_2CN^- , CH_3CHCN^- and $\text{CH}_2\text{CH}_2\text{CN}^-$ in the gas phase. A joint experimental and theoretical study. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 2466-2472. | 1.5 | 10 |
| 2465 | Substituent Effects on the Basicity of 3,7-Diazabicyclo[3.3.1]nonanes. <i>Journal of Organic Chemistry</i> , 2006, 71, 7155-7164. | 1.7 | 38 |
| 2466 | Matched Molecular Pairs as a Guide in the Optimization of Pharmaceutical Properties; a Study of Aqueous Solubility, Plasma Protein Binding and Oral Exposure. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 6672-6682. | 2.9 | 248 |
| 2467 | Single-Site Homogeneous and Heterogeneous Gold(III) Hydrogenation Catalysts: Mechanistic Implications. <i>Journal of the American Chemical Society</i> , 2006, 128, 4756-4765. | 6.6 | 161 |
| 2468 | Theoretical Comparison between Three-Point and Two-Point Binding Modes for Chiral Discrimination upon the N-Terminal Sequence of 310-Helix. <i>Polymer Journal</i> , 2006, 38, 432-441. | 1.3 | 8 |
| 2469 | Heterotropic Rearrangements: Hybrids of Electrocyclic and Sigmatropic Reactions. <i>Journal of Organic Chemistry</i> , 2006, 71, 3686-3695. | 1.7 | 47 |
| 2470 | Assessment of a Coulomb-attenuated exchange-correlation energy functional. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 558-562. | 1.3 | 437 |
| 2471 | Benchmark Study of DFT Functionals for Late-Transition-Metal Reactions. <i>Journal of Physical Chemistry A</i> , 2006, 110, 709-716. | 1.1 | 223 |
| 2472 | Cationic (η^1 -Allyl)-palladium Complexes as Feasible Intermediates in Catalyzed Reactions. <i>Organometallics</i> , 2006, 25, 3611-3618. | 1.1 | 30 |
| 2473 | Urea and Urea Nitrate Decomposition Pathways: A Quantum Chemistry Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2759-2770. | 1.1 | 33 |
| 2474 | Non-Aqueous Solvation of n-Octanol and Ethanol: Spectroscopic and Computational Studies. <i>Journal of Physical Chemistry B</i> , 2006, 110, 6325-6331. | 1.2 | 7 |
| 2475 | The Walden cycle revisited: a computational study of competitive ring closure to β - and γ -lactones. <i>Chemical Communications</i> , 2006, , 1106. | 2.2 | 9 |
| 2476 | Gas-Phase Ion Chemistry of BF ₃ /NH ₃ Mixtures. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12427-12433. | 1.1 | 5 |
| 2477 | THE PECULIAR ELECTRONIC STRUCTURE OF THE DI-METALLOCENE: THE EVIDENCE FOR THE STABILITY AND THE CHARACTER OF METAL-METAL BOND. <i>Journal of Theoretical and Computational Chemistry</i> , 2006, 05, 461-473. | 1.8 | 15 |
| 2478 | Local cation environments in the pyrope-grossular Mg ₃ Al ₂ Si ₃ O ₁₂ -Ca ₃ Al ₂ Si ₃ O ₁₂ garnet solid solution. <i>Physical Review B</i> , 2006, 74, . | 1.1 | 30 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 2479 | High electron affinities of bicyclo[n,n, 0]perfluoroalkanes. <i>Molecular Physics</i> , 2006, 104, 1311-1324. | 0.8 | 3 |
| 2480 | Mechanisms and Free Energies of Enzymatic Reactions. <i>Chemical Reviews</i> , 2006, 106, 3188-3209. | 23.0 | 355 |
| 2481 | Synthesis, Structural Studies, Theoretical Calculations, and Linear and Nonlinear Optical Properties of Terpyridyl Lanthanide Complexes: A New Evidence for the Contribution of f Electrons to the NLO Activity. <i>Journal of the American Chemical Society</i> , 2006, 128, 12243-12255. | 6.6 | 113 |
| 2482 | Gold as hydrogen: Structural and electronic properties and chemical bonding in $\text{Si}_3\text{Au}_3+\hat{\text{O}}\hat{\text{A}}^{\wedge}$ and comparisons to $\text{Si}_3\text{H}_3+\hat{\text{O}}\hat{\text{A}}^{\wedge}$. <i>Journal of Chemical Physics</i> , 2006, 125, 133204. | 1.2 | 75 |
| 2483 | Circular Dichroism Spectroscopy. , 0, , 265-304. | | 3 |
| 2484 | Relativistic Density Functional Theory Study of Dioxoactinide(VI) and -(V) Complexation with Alaskaphyrin and Related Schiff-Base Macrocyclic Ligands. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9486-9499. | 1.1 | 72 |
| 2485 | Task-Specific Ionic Liquid for Solubilizing Metal Oxides. <i>Journal of Physical Chemistry B</i> , 2006, 110, 20978-20992. | 1.2 | 412 |
| 2486 | Structural Characterization of POSS Siloxane Dimer and Trimer. <i>Chemistry of Materials</i> , 2006, 18, 1490-1497. | 3.2 | 51 |
| 2487 | Testing the TPSS meta-generalized-gradient-approximation exchange-correlation functional in calculations of transition states and reaction barriers. <i>Journal of Chemical Physics</i> , 2006, 125, 234104. | 1.2 | 46 |
| 2488 | Trinuclear Copper(II) Complexes Derived from Schiff-Base Ligands Based on a 6-Amino-6-deoxyglucopyranoside: Structural and Magnetic Characterization. <i>Inorganic Chemistry</i> , 2006, 45, 10066-10076. | 1.9 | 64 |
| 2489 | SCRF-DFT and NMR Comparison of Tetracycline and 5a,6-Anhydrotetracycline in Solution. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24766-24774. | 1.2 | 14 |
| 2490 | Monolaterol, the First Configurationally Assigned Phenylphenalenone Derivative with a Stereogenic Center at C-9, from <i>Monochoria elata</i> . <i>Journal of Natural Products</i> , 2006, 69, 1614-1617. | 1.5 | 17 |
| 2491 | Structure-Property Relationships in Push-Pull Amino/Cyanovinyl End-Capped Oligothiophenes: Quantum Chemical and Experimental Studies. <i>Journal of Organic Chemistry</i> , 2006, 71, 7509-7520. | 1.7 | 81 |
| 2492 | Woodward-Hoffmann rules in density functional theory: Initial hardness response. <i>Journal of Chemical Physics</i> , 2006, 125, 214101. | 1.2 | 72 |
| 2493 | Bonding analysis using localized relativistic orbitals: Water, the ultrarelativistic case and the heavy homologues H_2X ($\text{X}=\text{Te}, \text{Po}, \text{eka-Po}$). <i>Journal of Chemical Physics</i> , 2006, 124, 154307. | 1.2 | 37 |
| 2494 | Octopolar Chromophores Based on Donor- and Acceptor-Substituted 1,3,5-Tris(phenylethynyl)benzenes: Impact of meta-Conjugation on the Molecular and Electronic Structure by Means of Spectroscopy and Theory. <i>Journal of Physical Chemistry B</i> , 2006, 110, 19198-19206. | 1.2 | 31 |
| 2495 | Combined Quantum Chemical Density Functional Theory and Spectroscopic Raman and UV-vis-NIR Study of Oligothienoacenes with Five and Seven Rings. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5058-5065. | 1.1 | 39 |
| 2496 | Quantum Chemical and Statistical Rate Study of the Reaction of $\text{O}(^3\text{P})$ with Allene: O-Addition and H-Abstraction Channels. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12166-12176. | 1.1 | 24 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2497 | Exploration of Ground and Excited Electronic States of Aromatic and Quinoid S,S-Dioxide Terthiophenes. Complementary Systems for Enhanced Electronic Organic Materials. <i>Journal of the American Chemical Society</i> , 2006, 128, 10134-10144. | 6.6 | 55 |
| 2498 | Methane Activation by Laser-Ablated V, Nb, and Ta Atoms: Formation of CH ⁺ MH, CH ₂ MH ₂ , CH ⁺ MH ₃ , and (CH ₃) ₂ MH ₂ . <i>Journal of Physical Chemistry A</i> , 2006, 110, 3886-3902. | 1.1 | 41 |
| 2499 | Understanding the Origins of Remote Asymmetric Induction in the Boron Aldol Reactions of β^2 -Alkoxy Methyl Ketones. <i>Organic Letters</i> , 2006, 8, 4299-4302. | 2.4 | 67 |
| 2500 | Divinylphenylene-Bridged Diruthenium Complexes Bearing Ru(CO)Cl(PiPr ₃) ₂ Entities. <i>Organometallics</i> , 2006, 25, 3701-3712. | 1.1 | 107 |
| 2501 | A Triplet Mechanism for the Formation of Cyclobutane Pyrimidine Dimers in UV-Irradiated DNA. <i>Journal of Physical Chemistry B</i> , 2006, 110, 7556-7562. | 1.2 | 68 |
| 2502 | Polar Group Enhanced Gas-Phase Acidities of Carboxylic Acids: An Investigation of Intramolecular Electrostatic Interaction. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13405-13411. | 1.1 | 4 |
| 2503 | The Active Role of the Water Solvent in the Regioselective CO Hydrogenation of Unsaturated Aldehydes by [RuH ₂ (mtpms) _x] in Basic Media. <i>Organometallics</i> , 2006, 25, 5010-5023. | 1.1 | 52 |
| 2504 | Gas-Phase Structures, Rotational Barriers, and Conformational Properties of Hydroxyl and Mercapto Derivatives of Cyclohexa-2,5-dienone and Cyclohexa-2,5-dienthione. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8901-8911. | 1.1 | 8 |
| 2505 | Density Functional Calculations of ³ He Chemical Shift in Endohedral Helium Fullerenes: Neutral, Anionic, and Di-Helium Species. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12338-12341. | 1.1 | 29 |
| 2506 | Is NO ₃ Formed during the Decomposition of Nitramine Explosives?. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13974-13978. | 1.1 | 24 |
| 2507 | Computational Insights into the Mechanism of Radical Generation in B12-Dependent Methylmalonyl-CoA Mutase. <i>Journal of the American Chemical Society</i> , 2006, 128, 1287-1292. | 6.6 | 83 |
| 2508 | Rotational Tensors Calculated Using Hybrid Exchange-Correlation Functionals with the Optimized Effective Potential Approach. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 827-834. | 2.3 | 14 |
| 2509 | Intermolecular Association of Tetrahydrofuran-2-carboxylic Acid in Solution: A Vibrational Circular Dichroism Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10191-10200. | 1.1 | 47 |
| 2510 | Charge Penetration and the Origin of Large O-H Vibrational Red-Shifts in Hydrated-Electron Clusters, (H ₂ O) _n ⁻ . <i>Journal of the American Chemical Society</i> , 2006, 128, 13932-13939. | 6.6 | 59 |
| 2511 | Toward a Reversible Isolation of a C ₂₀ Fullerene Inside a Tetraarecalix[4]arene Dimer. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9405-9410. | 1.1 | 5 |
| 2512 | Density Functional Theory Studies of Actinide(III) Motexafins (An-Motex ₂₊ , An = Ac, Cm, Lr). Structure, Stability, and Comparison with Lanthanide(III) Motexafins. <i>Inorganic Chemistry</i> , 2006, 45, 3444-3451. | 1.9 | 30 |
| 2513 | Hydrogen Bonding in Substituted Formic Acid Dimers. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12623-12628. | 1.1 | 48 |
| 2514 | A Combined Experimental and Theoretical Study on the Effect of Doping and Interface Formation on Ppv ⁺ ether Copolymer. <i>Journal of Physical Chemistry B</i> , 2006, 110, 1141-1150. | 1.2 | 10 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2515 | Synthesis, Molecular Structure, and Reactivity of the Isolable Silylenoid with a Tricoordinate Silicon. <i>Journal of the American Chemical Society</i> , 2006, 128, 2784-2785. | 6.6 | 88 |
| 2516 | Electronic Structure, Bonding, Spectroscopy and Energetics of Fe-Dependent Nitrile Hydratase Active-Site Models. <i>Inorganic Chemistry</i> , 2006, 45, 17-36. | 1.9 | 29 |
| 2517 | Hydrogen Transfer between Sulfuric Acid and Hydroxyl Radical in the Gas Phase: Competition among Hydrogen Atom Transfer, Proton-Coupled Electron-Transfer, and Double Proton Transfer. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1982-1990. | 1.1 | 33 |
| 2518 | Carbosilane Dendrons as Solubilizers of Metal Complexes in Supercritical Carbon Dioxide. <i>Organometallics</i> , 2006, 25, 4138-4143. | 1.1 | 34 |
| 2519 | Theoretical Studies on Farnesyl Cation Cyclization: Pathways to Pentalenene. <i>Journal of the American Chemical Society</i> , 2006, 128, 6172-6179. | 6.6 | 119 |
| 2520 | Accuracy vs Time Dilemma on the Prediction of NMR Chemical Shifts: A Case Study (Chloropyrimidines). <i>Journal of Organic Chemistry</i> , 2006, 71, 3103-3110. | 1.7 | 15 |
| 2521 | Dimensionality Dependence of Optical Properties and Quantum Confinement Effects of Hydrogenated Silicon Nanostructures. <i>Journal of Physical Chemistry B</i> , 2006, 110, 21528-21535. | 1.2 | 12 |
| 2522 | Multicenter Bonding in Carbocations with Tetracoordinate Protons. <i>Journal of Physical Chemistry A</i> , 2006, 110, 3785-3789. | 1.1 | 19 |
| 2523 | Ligand Rearrangement Reactions of Cr(CO) ₆ in Alcohol Solutions: Experiment and Theory. <i>Journal of Physical Chemistry B</i> , 2006, 110, 996-1005. | 1.2 | 22 |
| 2524 | Allylic H-Abstraction Mechanism: The Potential Energy Surface of the Reaction of Propene with OH Radical. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1575-1586. | 2.3 | 66 |
| 2525 | Synthesis and Reactivity of Bis(alkoxyalkylidene)platinum(II) Complexes. <i>Organometallics</i> , 2006, 25, 5946-5954. | 1.1 | 27 |
| 2526 | Activation of Methane by the Iron Dimer Cation. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12501-12511. | 1.1 | 24 |
| 2527 | Theoretical and Experimental Studies on the Baeyer-Villiger Oxidation of Ketones and the Effect of α -Halo Substituents. <i>Journal of Organic Chemistry</i> , 2006, 71, 861-872. | 1.7 | 69 |
| 2528 | High-Level ab Initio Studies of Hydrogen Abstraction from Prototype Hydrocarbon Systems. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11160-11173. | 1.1 | 49 |
| 2529 | Oxidative Addition of the Chloromethane C-Cl Bond to Pd, an ab Initio Benchmark and DFT Validation Study. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 322-335. | 2.3 | 81 |
| 2530 | Structure and Bonding in Monomeric Iron(III) Complexes with Terminal Oxo and Hydroxo Ligands. <i>Inorganic Chemistry</i> , 2006, 45, 1732-1738. | 1.9 | 7 |
| 2531 | Ancistrocladinium A and B, the First N,C-Coupled Naphthyldihydroisoquinoline Alkaloids, from a Congolese <i>Ancistrocladus</i> Species. <i>Journal of Organic Chemistry</i> , 2006, 71, 9348-9356. | 1.7 | 80 |
| 2532 | Electronic Excited States of Si(100) and Organic Molecules Adsorbed on Si(100). <i>Journal of Physical Chemistry B</i> , 2006, 110, 1701-1710. | 1.2 | 25 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2533 | Activation of CH ₄ by Gas-Phase Mo ⁺ , and the Thermochemistry of Mo ⁺ ligand Complexes. Journal of Physical Chemistry A, 2006, 110, 8327-8338. | 1.1 | 40 |
| 2534 | Density Functional Study of the O ₂ Binding to [CuI(TPA)] ⁺ (TPA = Tris(2-pyridylmethyl)amine) in THF and EtCN. Inorganic Chemistry, 2006, 45, 1491-1497. | 1.9 | 10 |
| 2535 | Assessment of the Pairwise Additive Approximation and Evaluation of Many-Body Terms for Water Clusters. Journal of Physical Chemistry B, 2006, 110, 10595-10601. | 1.2 | 42 |
| 2536 | Quantum Chemical Characterization of the Bonding of N-Heterocyclic Carbenes to Cp ₂ MI Compounds [M = Ce(III), U(III)]. Inorganic Chemistry, 2006, 45, 9442-9447. | 1.9 | 33 |
| 2537 | Molecular Mechanical Devices Based on Quinone-pyrrole and Quinone-indole Dyads: A Computational Study. Journal of Physical Chemistry B, 2006, 110, 8158-8165. | 1.2 | 9 |
| 2538 | Assessment of Density Functionals for π Systems: Energy Differences between Cumulenes and Polyynes; Proton Affinities, Bond Length Alternation, and Torsional Potentials of Conjugated Polyenes; and Proton Affinities of Conjugated Schiff Bases. Journal of Physical Chemistry A, 2006, 110, 10478-10486. | 1.1 | 196 |
| 2539 | Stopped-Flow Kinetics of Tetrazine Cycloadditions; Experimental and Computational Studies toward Sequential Transition States. Journal of Physical Chemistry A, 2006, 110, 1288-1294. | 1.1 | 31 |
| 2540 | Structures and Reaction Mechanisms of Propene Oxide Isomerization on H-ZSM-5: An ONIOM Study. Journal of Physical Chemistry B, 2006, 110, 25950-25957. | 1.2 | 43 |
| 2541 | Mixed P ⁺ N and As ⁺ N Bis-Ylide Palladium Complexes: Cooperative Intramolecular Interactions, Conformational Preferences, and C-H Bond Activations. Organometallics, 2006, 25, 4653-4664. | 1.1 | 31 |
| 2542 | Experimental and Theoretical Study of the Vibrational Spectra of 12-Crown-4 Alkali Metal Cation Complexes. Journal of Physical Chemistry A, 2006, 110, 8676-8687. | 1.1 | 29 |
| 2543 | Quantum Chemical and Theoretical Kinetics Study of the O(3P) + C ₂ H ₂ Reaction: A Multistate Process. Journal of Physical Chemistry A, 2006, 110, 6696-6706. | 1.1 | 48 |
| 2544 | Density Functional Study of Electron Paramagnetic Resonance Parameters and Spin Density Distributions of Dicopper(I) Complexes with Bridging Azo and Tetrazine Radical-Anion Ligands. Journal of Physical Chemistry A, 2006, 110, 4021-4033. | 1.1 | 18 |
| 2545 | Stabilization of a Dialkylstannylene by Unusual B ⁺ H ⁻ ...Sn ⁺ Agostic-Type Interactions. A Structural, Spectroscopic, and DFT Study. Organometallics, 2006, 25, 1135-1143. | 1.1 | 35 |
| 2546 | Ortho Effect in the Bergman Cyclization: Electronic and Steric Effects in Hydrogen Abstraction by 1-Substituted Naphthalene 5,8-Diradicals. Journal of Physical Chemistry A, 2006, 110, 2517-2526. | 1.1 | 48 |
| 2547 | Reactions of tBuCp*P with Cyclooctatetraene-Supported Titanium Imido Complexes. Organometallics, 2006, 25, 3688-3700. | 1.1 | 14 |
| 2548 | Gate Effect of Vacancy-type Defect of Fullerene Cages on Metal-Atom Migrations in Metallofullerenes. Nano Letters, 2006, 6, 1389-1395. | 4.5 | 16 |
| 2549 | Hydrogen Bond Detection. Journal of Physical Chemistry A, 2006, 110, 4229-4237. | 1.1 | 62 |
| 2550 | Structure and properties of the Ni@Si ₁₂ cluster from all-electron ab initio calculations. Physical Review B, 2006, 73, . | 1.1 | 43 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2551 | DFT Calculations on the Protonation of Two 1,3-Butadiyne Units Fixed in Medium-Sized Rings. <i>Journal of Organic Chemistry</i> , 2006, 71, 5126-5135. | 1.7 | 6 |
| 2552 | Theoretical Insights, in the Liquid Phase, Into the Antioxidant Mechanism-Related Parameters in the 2-Monosubstituted Phenols. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11151-11159. | 1.1 | 30 |
| 2553 | Silicon Radicals in Silicon Oxynitride: A Theoretical ESR Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8637-8644. | 1.1 | 0 |
| 2554 | Highly Oxidized Ruthenium Organometallic Compounds. The Synthesis and One-Electron Electrochemical Oxidation of [Cp* <i>Ru</i> IVCl ₂ (S ₂ CR)] (Cp* = η^5 -C ₅ Me ₅ , R = NMe ₂ , NEt ₂ , O <i>i</i> Pr). <i>Organometallics</i> , 2006, 25, 6134-6141. | 1.1 | 16 |
| 2555 | EPR and ENDOR Study of Radiation-Induced Radical Formation in Purines: Sodium Inosine Crystals X-irradiated at 10 K. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6552-6562. | 1.1 | 4 |
| 2556 | Nonclassical Carbocations as C α -H Hydrogen Bond Donors. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4810-4816. | 1.1 | 41 |
| 2557 | Theoretical Rationale for Regioselection in Phosphine-Catalyzed Allenolate Additions to Acrylates, Imines, and Aldehydes. <i>Organic Letters</i> , 2006, 8, 3643-3646. | 2.4 | 143 |
| 2558 | Electronic Structure of Mononuclear Bis(1,2-diaryl-1,2-ethylenedithiolato)iron Complexes Containing a Fifth Cyanide or Phosphite Ligand: A Combined Experimental and Computational Study. <i>Inorganic Chemistry</i> , 2006, 45, 7877-7890. | 1.9 | 31 |
| 2559 | Computational Studies of Ethynyl- and Diethynyl-Expanded Tetrahedranes, Prismanes, Cubanones, and Adamantanones. <i>Journal of Organic Chemistry</i> , 2006, 71, 5105-5116. | 1.7 | 23 |
| 2560 | Conformational Stability of a Model Macrocyclic Tetraamide: An <i>ab Initio</i> Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4487-4494. | 1.1 | 7 |
| 2561 | Computational Study of 1,3-Dithiane 1,1-Dioxide (1,3-Dithiane Sulfone). Description of the Inversion Process and Manifestation of Stereoelectronic Effects on 1J _{C-H} Coupling Constants. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7703-7712. | 1.1 | 22 |
| 2562 | How Efficient Are the Hydrido-Bridged Diplatinum Catalysts in the Hydrosilylation, Hydrocyanation, and Hydroamination of Alkynes: A Theoretical Analysis of the Catalytic Cycles Employing Electronic Structure Calculation Methods. <i>Organometallics</i> , 2006, 25, 1696-1706. | 1.1 | 35 |
| 2563 | Gas-phase Ion Chemistry of BF ₃ /HN ₃ Mixtures: The First Observation of [BF _n N _x H _{n-1}] ⁺ (n = 1, 2; x = 1, 3) Ions. <i>Journal of Physical Chemistry B</i> , 2006, 110, 4492-4499. | 1.2 | 9 |
| 2564 | Quantum Chemical Study of Solvent and Substituent Effects on the 1,5-Hydride Shift in 2,6-Dimethyl-2-heptyl Cations. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1868-1874. | 1.1 | 21 |
| 2565 | Nature and Role of Bridged Carbonyl Intermediates in the Ultrafast Photoinduced Rearrangement of Ru ₃ (CO) ₁₂ . <i>Organometallics</i> , 2006, 25, 775-784. | 1.1 | 28 |
| 2566 | C α -H Oxidative Addition of Bisimidazolium Salts to Iridium and Rhodium Complexes, and N-Heterocyclic Carbene Generation. A Combined Experimental and Theoretical Study. <i>Organometallics</i> , 2006, 25, 1120-1134. | 1.1 | 96 |
| 2567 | Pathways and Rate Coefficients for the Decomposition of Vinyloxy and Acetyl Radicals. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5772-5781. | 1.1 | 74 |
| 2568 | Ortho Effect in the Bergman Cyclization: Comparison of Experimental Approaches and Dissection of Cycloaromatization Kinetics. <i>Journal of Organic Chemistry</i> , 2006, 71, 962-975. | 1.7 | 77 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2569 | Phylloquinone and Related Radical Anions Studied by Pulse Electron Nuclear Double Resonance Spectroscopy at 34 GHz and Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11549-11560. | 1.2 | 34 |
| 2570 | Rate-Determining Cooperative Effects of Bimolecular Reactions in Solution. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13290-13294. | 1.1 | 4 |
| 2571 | Pseudo-Two-Dimensional Structures (HXYH) ₃ n ₂ H ₆ n (XY = GaN, SiC, GeC, SiSi, or GeGe; n = 1-3): A Density Functional Characterization of Structures and Energetics. <i>Journal of Physical Chemistry A</i> , 2006, 110, 494-502. | 1.1 | 4 |
| 2572 | A Combined Density Functional Theory and Coupled Cluster Method Investigation of the Structural Properties and Stabilities of Radical CH ₂ CP and Its Isomers. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2411-2420. | 1.1 | 1 |
| 2573 | Torsional Anharmonicity in the Conformational Analysis of ¹² -d-Galactose. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3485-3492. | 1.2 | 11 |
| 2574 | Theoretical Models on the Cu ₂ O ₂ Torture Track: A Mechanistic Implications for Oxytyrosinase and Small-Molecule Analogues. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1991-2004. | 1.1 | 179 |
| 2575 | Aromaticity and Möbius Antiaromaticity in Monocyclic [11]Annulenic Cations. <i>Journal of Organic Chemistry</i> , 2006, 71, 9271-9282. | 1.7 | 23 |
| 2576 | Pd _n CO (n = 1,2): Accurate Ab Initio Bond Energies, Geometries, and Dipole Moments and the Applicability of Density Functional Theory for Fuel Cell Modeling. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24030-24046. | 1.2 | 45 |
| 2577 | Tetracoordinate Carbon as a Nucleophile? Interconversion of Carbenium Ions with Carbonium Ions Possessing Nearly Square-Pyramidal Pentacoordinate Carbons. <i>Journal of Organic Chemistry</i> , 2006, 71, 645-654. | 1.7 | 22 |
| 2578 | Photoexcitation of Dinucleoside Radical Cations: A Time-Dependent Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24181-24188. | 1.2 | 45 |
| 2579 | CB ₁₁ Me ₁₁ Boronium Ylides: Carba-closo-dodecaboranes with a Naked Boron Vertex. <i>Journal of the American Chemical Society</i> , 2006, 128, 6089-6100. | 6.6 | 37 |
| 2580 | Hybrid Organic Semiconductors Including Chalcogen Atoms in π -Conjugated Skeletons. Tuning of Optical, Redox, and Vibrational Properties by Heavy Atom Conjugation. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7422-7430. | 1.1 | 25 |
| 2581 | On the Structure and Chemical Bonding of Tri-Tungsten Oxide Clusters W ₃ O _n - and W ₃ O _n (n = 7-10): A Potential Molecular Model for O-Deficient Defect Sites in Tungsten Oxides. <i>Journal of Physical Chemistry A</i> , 2006, 110, 85-92. | 1.1 | 83 |
| 2582 | Insight into Selected Reactions in Low-Temperature Dimethyl Ether Combustion from Born-Oppenheimer Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1393-1407. | 1.1 | 18 |
| 2583 | Theoretical Investigation of the Selective CC Hydrogenation of Unsaturated Aldehydes Catalyzed by [{RuCl ₂ (mtpmms) ₂ } ₂] in Acidic Media. <i>Organometallics</i> , 2006, 25, 862-872. | 1.1 | 27 |
| 2584 | Assessment of Model Chemistries for Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1009-1018. | 2.3 | 214 |
| 2585 | Density Functional Theory for Charge Transfer: The Nature of the N-Bands of Porphyrins and Chlorophylls Revealed through CAM-B3LYP, CASPT2, and SAC-CI Calculations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 15624-15632. | 1.2 | 315 |
| 2586 | Solvent Effects on Raman Optical Activity Spectra Calculated Using the Polarizable Continuum Model. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2807-2815. | 1.1 | 59 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2587 | Density Functional for Spectroscopy: No Long-Range Self-Interaction Error, Good Performance for Rydberg and Charge-Transfer States, and Better Performance on Average than B3LYP for Ground States. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13126-13130. | 1.1 | 1,140 |
| 2588 | Modeling Subtype-Selective Agonists Binding with $\alpha 4\beta 2$ and $\alpha 7$ Nicotinic Acetylcholine Receptors: Effects of Local Binding and Long-Range Electrostatic Interactions. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 7661-7674. | 2.9 | 46 |
| 2589 | Vibronic absorption, fluorescence, and phosphorescence spectra of psoralen: a quantum chemical investigation. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 2133. | 1.3 | 50 |
| 2590 | Efficient Intermolecular [2 + 2 + 2] Alkyne Cyclootrimerization in Aqueous Medium Using a Ruthenium(IV) Precatalyst. <i>Journal of the American Chemical Society</i> , 2006, 128, 15094-15095. | 6.6 | 94 |
| 2591 | On the art of computing the IR spectra of molecules in the condensed phase. , 2006, , 159-177. | | 6 |
| 2592 | Diagnostics for specific PAHs in the far-IR: searching neutral naphthalene and anthracene in the Red Rectangle. <i>Astronomy and Astrophysics</i> , 2006, 456, 161-169. | 2.1 | 42 |
| 2593 | Theoretical Study of Electronic Structures of [Peroxo]porphyrinato]manganate $[Mn(P)(O_2)]^{2-}$ Anion. <i>Bulletin of the Chemical Society of Japan</i> , 2006, 79, 1201-1210. | 2.0 | 5 |
| 2594 | Electron Transfer Reactions in Laser Desorption/Ionization and Matrix-Assisted Laser Desorption/Ionization: Factors Influencing Matrix and Analyte Ion Intensities. <i>European Journal of Mass Spectrometry</i> , 2006, 12, 345-358. | 0.5 | 36 |
| 2595 | DFT Calculations of Cubane-Type $Mo_2Ru_2S_4$ Clusters. Stability of a Possible Dinitrogen Cluster and an Isolable Acetonitrile Cluster. <i>Bulletin of the Chemical Society of Japan</i> , 2006, 79, 53-58. | 2.0 | 6 |
| 2596 | A study of the electronic and structural properties of C_{28} and $C_{16}N_{12}$. <i>Molecular Physics</i> , 2006, 104, 319-323. | 0.8 | 2 |
| 2598 | 2-Formylbenzotrile. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2006, 62, o307-o309. | 0.4 | 1 |
| 2599 | The one-electron oxidation of $[HCCOCC]^{+}$ to form neutral HCCOCC, and the subsequent rearrangement of HCCOCC to form HCCCO. An experimental and computational study. <i>Rapid Communications in Mass Spectrometry</i> , 2006, 20, 577-582. | 0.7 | 1 |
| 2600 | Bonding energetics in clusters formed by cesium salts: a study by collision-induced dissociation and density functional theory. <i>Rapid Communications in Mass Spectrometry</i> , 2006, 20, 2057-2062. | 0.7 | 11 |
| 2601 | Solid-Phase Synthesis and Structural Study of Substituted 1,4,5,6-Tetrahydro-6-oxopyridine-3-carboxylic Acids. <i>QSAR and Combinatorial Science</i> , 2006, 25, 921-927. | 1.5 | 11 |
| 2602 | Use of vibrational spectroscopy to study protein and DNA structure, hydration, and binding of biomolecules: A combined theoretical and experimental approach. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1160-1198. | 1.0 | 73 |
| 2603 | Potential energy surface of thionylimide. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1237-1249. | 1.0 | 11 |
| 2604 | Computational study of the synthesis of benzoin derivatives from benzil. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1596-1610. | 1.0 | 1 |
| 2605 | Theoretical study of the magnetic exchange coupling behavior substituting Cr(III) with Mo(III) in cyano-bridged transition metal complexes. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1551-1560. | 1.0 | 12 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2606 | Ab initio and DFT study of Y3+ hydration. International Journal of Quantum Chemistry, 2006, 106, 2236-2244. | 1.0 | 8 |
| 2607 | Ab initio MO study of potential energy surface of NH2 with CN reaction. International Journal of Quantum Chemistry, 2006, 106, 1827-1843. | 1.0 | 6 |
| 2608 | Singlet-triplet gaps and insertion reactions of aminocyanocarbenes: A computational study of hydrogen cyanide covalent dimers. International Journal of Quantum Chemistry, 2006, 106, 2379-2389. | 1.0 | 6 |
| 2609 | Theoretical and experimental study of aparisthman: A natural product with anti-ulcer activity. International Journal of Quantum Chemistry, 2006, 106, 2706-2713. | 1.0 | 8 |
| 2610 | Note on the calculation of analytical Hessians in the zeroth-order regular approximation (ZORA). International Journal of Quantum Chemistry, 2006, 106, 2525-2528. | 1.0 | 7 |
| 2611 | Local minima conformations of the Sc3N @C80 endohedral complex: Ab initio quantum chemical study and suggestions for experimental verification. International Journal of Quantum Chemistry, 2006, 106, 2975-2980. | 1.0 | 16 |
| 2612 | Application of electronic structure and transition state theory: Reaction of hydrogen with silicon radicals. International Journal of Quantum Chemistry, 2006, 106, 3149-3159. | 1.0 | 3 |
| 2613 | An integrated approach to the study of intramolecular hydrogen bonds in malonaldehyde enol derivatives and naphthazarin: trend in energetic versus geometrical consequences. Journal of Physical Organic Chemistry, 2006, 19, 425-444. | 0.9 | 94 |
| 2614 | Theory of excitation transfer in coupled nanostructures from quantum dots to light harvesting complexes. Physica Status Solidi (B): Basic Research, 2006, 243, 2302-2310. | 0.7 | 48 |
| 2615 | Use of pyridine CH(D) vibrations for the study of Lewis acidity of metal oxides. Applied Catalysis A: General, 2006, 307, 98-107. | 2.2 | 47 |
| 2616 | Theoretical investigation of catalytic HCO3 ⁻ hydrogenation in aqueous solutions. Catalysis Today, 2006, 115, 53-60. | 2.2 | 57 |
| 2617 | Biomimetic Facially Amphiphilic Antibacterial Oligomers with Conformationally Stiff Backbones. Chemistry and Biology, 2006, 13, 427-435. | 6.2 | 74 |
| 2618 | Effects of strong electron correlations in Ti8C12 Met-Car. Chemical Physics, 2006, 326, 97-106. | 0.9 | 8 |
| 2619 | Ab initio quantum chemical studies on the reactions of CF3O2 with OH. Chemical Physics, 2006, 327, 10-14. | 0.9 | 18 |
| 2620 | A density functional study on iodine dioxide-water complexes. Chemical Physics, 2006, 328, 165-172. | 0.9 | 8 |
| 2621 | Free tetra- and hexa-coordinated platinum-cyanide dianions, and : A combined photodetachment photoelectron spectroscopic and theoretical study. Chemical Physics, 2006, 329, 230-238. | 0.9 | 22 |
| 2622 | Structural features of neutral and protonated galanthamine: A crystallographic database and computational investigation. Chemical Physics, 2006, 328, 307-317. | 0.9 | 8 |
| 2623 | Structure of small TiCn clusters: A theoretical study. Chemical Physics, 2006, 330, 431-440. | 0.9 | 33 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2624 | Conformational structures and optical rotation of serine and cysteine. Chemical Physics Letters, 2006, 418, 1-10. | 1.2 | 5 |
| 2625 | The lowest quartet electronic states of MnC. Chemical Physics Letters, 2006, 417, 334-340. | 1.2 | 8 |
| 2627 | Interpolation density values on a cartesian grid: Improving the efficiency of Lebedev based numerical integration in Kohn-Sham density functional algorithms. Chemical Physics Letters, 2006, 418, 490-495. | 1.2 | 11 |
| 2628 | The importance of water clusters (H ₂ O) _n (n=2, 3, 4) in the reaction of Criegee intermediate with water in the atmosphere. Chemical Physics Letters, 2006, 419, 479-485. | 1.2 | 73 |
| 2629 | The application of CAM-B3LYP to the charge-transfer band problem of the zincbacteriochlorin-bacteriochlorin complex. Chemical Physics Letters, 2006, 420, 106-109. | 1.2 | 256 |
| 2630 | Structure of binary titanium-carbon ions: A theoretical study of TiC^+ . Chemical Physics Letters, 2006, 420, 110-113. | 1.2 | 4 |
| 2631 | The molecular structure of Roesky's sulfoxide. Another computational challenge. Chemical Physics Letters, 2006, 423, 422-426. | 1.2 | 8 |
| 2632 | Density-functional-theory study of the electric-field-induced second harmonic generation (EFISHG) of push-pull phenylpolyenes in solution. Chemical Physics Letters, 2006, 425, 267-272. | 1.2 | 99 |
| 2633 | Coexistence of metastable nitric acid dihydrates: A molecular level contribution to understanding the formation of polar stratospheric clouds crystals. Chemical Physics Letters, 2006, 426, 20-25. | 1.2 | 7 |
| 2634 | Performance of various density functionals for the hydrogen bonds in DNA base pairs. Chemical Physics Letters, 2006, 426, 415-421. | 1.2 | 149 |
| 2635 | Terahertz spectroscopy of 7-azaindole clusters in solution. Chemical Physics Letters, 2006, 429, 405-409. | 1.2 | 18 |
| 2636 | Predicted IR spectra of Ti ₈ C ₁₂ and TiC^+ . Chemical Physics Letters, 2006, 429, 410-413. | 1.2 | 7 |
| 2637 | Theoretical study of the reactivity of 4d transition metal ions with N ₂ O. Chemical Physics Letters, 2006, 430, 265-270. | 1.2 | 21 |
| 2638 | Theoretical study of carbon dioxide-carbon monoxide conversion by La ⁺ , Hf ⁺ and Ta ⁺ . Chemical Physics Letters, 2006, 431, 39-44. | 1.2 | 21 |
| 2639 | A B3LYP study of proton transfer path within a complex of benzene radical cation and water cluster. Chemical Physics Letters, 2006, 432, 22-26. | 1.2 | 5 |
| 2640 | Parity-violating effects in electron spin resonance g-tensors. Chemical Physics Letters, 2006, 433, 37-42. | 1.2 | 4 |
| 2641 | Structural investigation of lithium iodide in liquid dimethyl sulfoxide: Comparison between experiment and computation. Chemical Physics, 2006, 321, 100-110. | 0.9 | 19 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2642 | The adsorption of NO ₂ on (9,0) and (10,0) carbon nanotubes. <i>Chemical Physics</i> , 2006, 323, 511-518. | 0.9 | 41 |
| 2643 | Mixing of electronic states in molybdenum complexes involved in nitrogen activation. <i>Chemical Physics</i> , 2006, 324, 202-209. | 0.9 | 9 |
| 2644 | Synthetic and theoretical study on proline-catalyzed Knoevenagel condensation in ionic liquid. <i>Journal of Molecular Catalysis A</i> , 2006, 253, 212-221. | 4.8 | 68 |
| 2645 | ¹ H NMR and DFT studies of steric effects on intermolecular C-H...O hydrogen bonding in solution. <i>Journal of Molecular Structure</i> , 2006, 789, 43-51. | 1.8 | 8 |
| 2646 | Raman experimental and DFT theoretical studies on the adsorption behavior of benzoic acid on silver nanoparticles. <i>Journal of Molecular Structure</i> , 2006, 789, 157-161. | 1.8 | 15 |
| 2647 | Polyamines. I. Spectroscopic properties of N,N-bis-(phthalimidopropyl)-N-propylamine and supramolecular interactions in its crystals. <i>Journal of Molecular Structure</i> , 2006, 791, 137-143. | 1.8 | 24 |
| 2648 | X-ray and ab initio studies of the structure and vibrational spectra of 4-carboxy-1-methylpyridinium chloride. <i>Journal of Molecular Structure</i> , 2006, 797, 66-81. | 1.8 | 16 |
| 2649 | An experimental and theoretical study on the adsorption behaviors of MHBA ions on silver nano-particles. <i>Journal of Molecular Structure</i> , 2006, 797, 40-43. | 1.8 | 9 |
| 2650 | QM/MM and classical molecular dynamics simulation of histidine-tagged peptide immobilization on nickel surface. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2006, 423, 84-91. | 2.6 | 19 |
| 2651 | Synthesis, characterization, structure and luminescence studies of dinuclear gold(I) alkynyls of bis(diphenylphosphino)alkyl- and aryl-amines. <i>Inorganica Chimica Acta</i> , 2006, 359, 3639-3648. | 1.2 | 28 |
| 2652 | Accurate predictions of the EPR parameters in planar cobalt(II) complexes by hybrid density functional theory. <i>Inorganica Chimica Acta</i> , 2006, 359, 3865-3870. | 1.2 | 6 |
| 2653 | Synthesis and characterization of platinum(IV) complexes with N,S and S,S heterocyclic ligands. <i>Inorganica Chimica Acta</i> , 2006, 359, 4326-4334. | 1.2 | 32 |
| 2654 | Ligation of Be ⁺ and Mg ⁺ to NF ₃ : Structure, stability, and thermochemistry of the Be ⁺ (NF ₃) and Mg ⁺ (NF ₃) complexes. <i>International Journal of Mass Spectrometry</i> , 2006, 255-256, 11-19. | 0.7 | 4 |
| 2655 | An ¹¹ B NMR spectroscopy investigation of the mechanism of the reduction of nitriles by BH ₃ ·SMe ₂ . <i>Polyhedron</i> , 2006, 25, 2730-2736. | 1.0 | 12 |
| 2656 | Syntheses and structures of lithiated sulfones Li[CR(R ²)SO ₂ Ph] ← C versus O bound lithium. [{"Li{CH(Me)SO ₂ Ph}(thf)} ⁺] ⁻ ← The structure of a C-bound derivative. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 2358-2367. | 0.8 | 22 |
| 2657 | Synthetic, spectral and catalytic activity studies of ruthenium bipyridine and terpyridine complexes: Implications in the mechanism of the ruthenium(pyridine-2,6-bisoxazoline)(pyridine-2,6-dicarboxylate)-catalyzed asymmetric epoxidation of olefins utilizing H ₂ O ₂ . <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4419-4433. | 0.8 | 47 |
| 2658 | Nucleus-independent chemical shift (NICS) profiles in a series of monocyclic planar inorganic compounds. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4359-4366. | 0.8 | 155 |
| 2659 | Electronic differentiations in palladium-catalyzed allylic substitutions. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4508-4513. | 0.8 | 20 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2660 | Computational studies on the copper(II) catalyzed Michael reaction. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4474-4479. | 0.8 | 7 |
| 2661 | Computational study of the transmetalation process in the Suzuki-Miyaura cross-coupling of aryls. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4459-4466. | 0.8 | 140 |
| 2662 | The mechanism of transition metal catalyzed carbonylation of allyl halides: A theoretical investigation. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4498-4507. | 0.8 | 9 |
| 2663 | Ethylene addition to OsO ₃ (CH ₂) – A theoretical study. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4467-4473. | 0.8 | 13 |
| 2664 | The mechanism of ethylene polymerization by nickel salicylaldehyde catalysts – Agostic interactions and their kinetic isotope effects. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4379-4385. | 0.8 | 21 |
| 2665 | Structure and vibrations of Ga _n N _n (n=3–10) clusters. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 63, 272-275. | 2.0 | 2 |
| 2666 | IR-SERS study and theoretical analogue on the adsorption behavior of pyridine carboxylic acid on silver nanoparticles. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 63, 614-618. | 2.0 | 16 |
| 2667 | The role of structured water in the calibration and interpretation of theoretical IR spectra. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 65, 324-332. | 2.0 | 2 |
| 2668 | Modelling of UV-molecular spectra of several bis-pyrazolopyridines derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 65, 511-516. | 2.0 | 1 |
| 2669 | FT-Raman and FT-IR spectra, ab initio and density functional studies of 3,4-dichlorobenzyl alcohol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 65, 826-832. | 2.0 | 15 |
| 2670 | An experimental and theoretical study on the interaction of PHBA ions and H ₂ O molecules. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 65, 930-934. | 2.0 | 0 |
| 2671 | Density functional theory and Hartree-Fock studies: Geometry, vibrational frequencies and electronic properties of Anderson-type heteropolyanion, [XM ₆ O ₂₄] ⁿ⁻ (X=Te, VI, VII and M=Mo, W) and [SbVW ₆ O ₂₄] ⁷⁻ . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 65, 1104-1111. | 2.0 | 17 |
| 2672 | Electron capture dissociation of peptides metalated with alkaline-earth metal ions. <i>Journal of the American Society for Mass Spectrometry</i> , 2006, 17, 757-771. | 1.2 | 54 |
| 2673 | Ab initio and DFT investigation of fluorinated methyl hydroperoxides: Structures, rotational barriers, and thermochemical properties. <i>Journal of Fluorine Chemistry</i> , 2006, 127, 54-62. | 0.9 | 11 |
| 2674 | A DFT overview of high-valent iron, cobalt and nickel tetraamidomacrocyclic ligand (TAML) complexes: The end of innocence?. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 620-626. | 1.5 | 12 |
| 2675 | Conformational analysis of bis(trigonelline) hydrochloride, perchlorate and their monohydrates by the B3LYP calculations, X-ray diffraction and vibrational spectra. <i>Journal of Molecular Structure</i> , 2006, 784, 98-108. | 1.8 | 26 |
| 2676 | Structure and UV-vis spectroscopy of roussin black salt [Fe ₄ S ₃ (NO) ₇] ³⁻ . <i>Journal of Molecular Structure</i> , 2006, 785, 68-75. | 1.8 | 28 |
| 2677 | Crystal and molecular structure of 3-(2-amino-pyridinium)-propionate monohydrate. <i>Journal of Molecular Structure</i> , 2006, 786, 25-32. | 1.8 | 16 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2678 | Hydrogen bonds and conformational analysis of bis(1-methylisonicotinate) hydrochloride monohydrate by X-ray diffraction, vibrational spectra and B3LYP calculations. <i>Journal of Molecular Structure</i> , 2006, 794, 46-53. | 1.8 | 22 |
| 2679 | Synthesis, properties and molecular structure of a novel dicyanoheptafulvene derivative, 4- β -dicyanomethylidenedispiro[cyclohexane-1, 1'- β -(1,4,7-trihydrocyclopenta[f]azulene)-7 β ,1 β -cyclohexane]. <i>Tetrahedron</i> , 2006, 62, 586-593. | | |
| 2680 | A straightforward synthesis and structure of unprecedented iminium salts of dihydropyrido[3,2-e][1,3]thiazines. <i>Tetrahedron</i> , 2006, 62, 1365-1371. | 1.0 | 16 |
| 2681 | New chiral lithium aluminum hydrides based on biphenyl-2,2'-bisfenchol (BIFOL): structural analyses and enantioselective reductions of aryl alkyl ketones. <i>Tetrahedron</i> , 2006, 62, 3704-3709. | 1.0 | 15 |
| 2682 | A computational study of halomethylithium carbenoid mixed aggregates with lithium halides and lithium methoxide. <i>Tetrahedron</i> , 2006, 62, 10821-10828. | 1.0 | 47 |
| 2683 | Correlation of calculated halonium ion structures with product distributions from fluorine substituted terminal alkenes. <i>Tetrahedron</i> , 2006, 62, 11608-11617. | 1.0 | 7 |
| 2684 | The combination of deconvolution and density functional theory for the mid-infrared vibrational spectra of stable and unstable rhodium carbonyl clusters. <i>Vibrational Spectroscopy</i> , 2006, 41, 101-111. | 1.2 | 28 |
| 2685 | Infrared, Raman spectra and DFT calculations of chlorine substituted anilines. <i>Vibrational Spectroscopy</i> , 2006, 42, 397-402. | 1.2 | 41 |
| 2686 | Chemoenzymatic synthesis of enantiomerically pure tricyclic benzomorphan analogues. <i>Tetrahedron: Asymmetry</i> , 2006, 17, 3046-3050. | 1.8 | 10 |
| 2687 | Vibrational circular dichroism DFT study on bicyclo[3.3.0]octane derivatives. <i>Tetrahedron: Asymmetry</i> , 2006, 17, 3203-3218. | 1.8 | 12 |
| 2688 | Synthesis of 2H-pyrroles via the 1,3-dipolar cycloaddition reaction of nitrile ylides with acrylamides. <i>Tetrahedron Letters</i> , 2006, 47, 477-481. | 0.7 | 14 |
| 2689 | A theoretical study of ethylene dehydrogenation by bare Niobium atom and cation. <i>Computational and Theoretical Chemistry</i> , 2006, 762, 25-31. | 1.5 | 14 |
| 2690 | Computational electrochemistry of aqueous two-electron reduction potentials of some amino-9,10-anthraquinone derivatives. <i>Computational and Theoretical Chemistry</i> , 2006, 758, 71-74. | 1.5 | 20 |
| 2691 | Urea parametrization for molecular dynamics simulations. <i>Computational and Theoretical Chemistry</i> , 2006, 758, 139-148. | 1.5 | 24 |
| 2692 | Theoretical study on the reaction mechanism of bis-addition of methyl azide to C60. <i>Computational and Theoretical Chemistry</i> , 2006, 760, 45-52. | 1.5 | 5 |
| 2693 | Computational study of pyrylium cation-water complexes: hydrogen bonds, resonance effects, and aromaticity. <i>Computational and Theoretical Chemistry</i> , 2006, 760, 59-73. | 1.5 | 17 |
| 2694 | Ab initio and density functional study of spectroscopic properties of CuO and CuS. <i>Computational and Theoretical Chemistry</i> , 2006, 761, 17-20. | 1.5 | 16 |
| 2695 | Ab initio quantum chemical studies of reaction mechanism for CH ₂ CO with NCO. <i>Computational and Theoretical Chemistry</i> , 2006, 760, 131-140. | 1.5 | 12 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 2696 | Scaling factors for vibrational frequencies and zero-point vibrational energies of some recently developed exchange-correlation functionals. <i>Computational and Theoretical Chemistry</i> , 2006, 760, 189-192. | 1.5 | 108 |
| 2697 | Quantum computations of the UV-visible spectra of uric acid and its anions. <i>Computational and Theoretical Chemistry</i> , 2006, 761, 203-207. | 1.5 | 11 |
| 2698 | Theoretical study on the reaction mechanism of bis-addition of methyl azide to C60 (II). <i>Computational and Theoretical Chemistry</i> , 2006, 765, 53-59. | 1.5 | 2 |
| 2699 | DFT-molecular modeling analysis of C-H...N and C-H...S hydrogen bond type interactions in selected platinum-purine/pyrimidine complexes. <i>Computational and Theoretical Chemistry</i> , 2006, 766, 61-72. | 1.5 | 16 |
| 2700 | Theoretical investigation of the reactivity in the C-F bond activation of CH3F by La+ in the gas phase. <i>Computational and Theoretical Chemistry</i> , 2006, 765, 27-34. | 1.5 | 18 |
| 2701 | Concerning the precision of standard density functional programs: Gaussian, Molpro, NWChem, Q-Chem, and Gamess. <i>Computational and Theoretical Chemistry</i> , 2006, 768, 175-181. | 1.5 | 197 |
| 2702 | What is the best theoretical method to study molybdenum dithiolene complexes?. <i>Computational and Theoretical Chemistry</i> , 2006, 773, 59-70. | 1.5 | 20 |
| 2703 | Mechanism for the gas-phase reaction between N3 and NO2: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2006, 801, 39-45. | 1.5 | 1 |
| 2704 | The Azido Gauche Effect: Implications for the Conformation of Azidoproline. <i>Journal of the American Chemical Society</i> , 2006, 128, 14697-14703. | 6.6 | 112 |
| 2705 | A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. <i>Journal of Chemical Physics</i> , 2006, 125, 194101. | 1.2 | 4,175 |
| 2706 | Hybrid Density Functional Methods Empirically Optimized for the Computation of ¹³ C and ¹ H Chemical Shifts in Chloroform Solution. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1085-1092. | 2.3 | 151 |
| 2707 | Theoretical Studies on the Bifunctionality of Chiral Thiourea-Based Organocatalysts: Competing Routes to C-C Bond Formation. <i>Journal of the American Chemical Society</i> , 2006, 128, 13151-13160. | 6.6 | 408 |
| 2708 | Donor-Stabilized Silyl Cations. 11. Bis-Zwitterionic Penta- and Hexacoordinate Silicon Dichelate Complexes Derived from (ClCH ₂) ₂ SiCl ₂ through Double Internal Displacement of Chloride. <i>Organometallics</i> , 2006, 25, 5416-5423. | 1.1 | 14 |
| 2709 | Kinetics of Triscarbonato Uranyl Reduction by Aqueous Ferrous Iron: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9691-9701. | 1.1 | 34 |
| 2710 | Effect of Structure in Benzaldehyde Oximes on the Formation of Aldehydes and Nitriles under Photoinduced Electron-Transfer Conditions. <i>Journal of Organic Chemistry</i> , 2006, 71, 7785-7792. | 1.7 | 11 |
| 2711 | Modeling the Kinetics of Bimolecular Reactions. <i>Chemical Reviews</i> , 2006, 106, 4518-4584. | 23.0 | 533 |
| 2712 | The Guanine Cation Radical: Investigation of Deprotonation States by ESR and DFT. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24171-24180. | 1.2 | 133 |
| 2713 | Ionic Liquids from Car Parrinello Simulations, Part I: Liquid AlCl ₃ . <i>Journal of Physical Chemistry B</i> , 2006, 110, 11475-11480. | 1.2 | 31 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2714 | Theoretical Investigation of Enolborane Addition to $\hat{I}\pm$ -Heteroatom-Substituted Aldehydes. Relevance of the Cornforth and Polar Felkinâ€™Anh Models for Asymmetric Induction. <i>Journal of the American Chemical Society</i> , 2006, 128, 2920-2930. | 6.6 | 91 |
| 2715 | Role of carbon clusters in pyrolysis of iodomethanes. <i>Russian Journal of General Chemistry</i> , 2006, 76, 245-250. | 0.3 | 0 |
| 2716 | Synthesis, structure, and properties of phosphorus-containing bis(amidrazones). <i>Russian Journal of General Chemistry</i> , 2006, 76, 1219-1225. | 0.3 | 5 |
| 2717 | Quantum-chemical study of nitrosonium complexes derived from nitrogen-containing heterocycles. <i>Russian Journal of Organic Chemistry</i> , 2006, 42, 1551-1562. | 0.3 | 0 |
| 2718 | Ultraviolet Absorption Spectra of Substituted Phenols: A Computational Studyâ€™. <i>Photochemistry and Photobiology</i> , 2006, 82, 324. | 1.3 | 30 |
| 2719 | A Theoretical Elucidation on the Solvent-dependent Photosensitive Behaviors of C60. <i>Photochemistry and Photobiology</i> , 2006, 82, 798. | 1.3 | 30 |
| 2720 | Semiempirical hybrid density functional with perturbative second-order correlation. <i>Journal of Chemical Physics</i> , 2006, 124, 034108. | 1.2 | 2,729 |
| 2721 | Synthesis and structure elucidation of oxidative coupling products of 2-hydroxy-1,4-naphthoquinones. <i>Russian Chemical Bulletin</i> , 2006, 55, 301-305. | 0.4 | 7 |
| 2722 | NMR parameters of the tetrahedrane $[\text{Fe}_2(\text{CO})_6(\hat{I}\frac{1}{4}\text{-SNH})]$, studied by experiment and DFT. <i>Structural Chemistry</i> , 2006, 17, 79-83. | 1.0 | 10 |
| 2723 | Reaction mechanism of the direct carboxylation of methanol to dimethylcarbonate: experimental and theoretical studies. <i>Topics in Catalysis</i> , 2006, 40, 71-81. | 1.3 | 50 |
| 2724 | Ab initio study of the structure of enolic and ketonic forms of \hat{I}^2 -diketones with the general formula $\text{R}\hat{\alpha}\epsilon^3\text{COCH}_2\text{COR}\hat{\alpha}\epsilon^2$ ($\text{R}\hat{\alpha}\epsilon^2$ and $\text{R}\hat{\alpha}\epsilon^3$ = H, CH ₃ , CF ₃). <i>Journal of Structural Chemistry</i> , 2006, 47, 220-231. | 0.3 | 12 |
| 2725 | DFT study of the structural characteristics of the yttrium(3+) aqua ion. <i>Journal of Structural Chemistry</i> , 2006, 47, 413-419. | 0.3 | 9 |
| 2726 | Conformational analysis of 2,3-dihydro-3-O-(1,4-naphthoquinon-2-yl)-2-oxo-1,4-naphthoquinone derivatives by the density functional method and IR spectroscopy. <i>Journal of Applied Spectroscopy</i> , 2006, 73, 640-649. | 0.3 | 0 |
| 2727 | Calculation of frequencies of normal vibrations and interpretation of IR spectra for 2,3-dihydro-3-O-(1,4-naphthoquinon-2-yl)-2-oxo-1,4-naphthoquinone derivatives. <i>Journal of Applied Spectroscopy</i> , 2006, 73, 798-806. | 0.3 | 4 |
| 2728 | Experimental (FT-IR) and theoretical (DFT) studies on the adsorption behavior of p-nitroaniline (PNA) on gold nanoparticales. <i>Journal of Nanoparticle Research</i> , 2006, 8, 761-767. | 0.8 | 17 |
| 2729 | Umpolung catalysts: comparative assessments on reactivities. <i>Journal of Molecular Modeling</i> , 2006, 12, 591-595. | 0.8 | 27 |
| 2730 | The formation of endo-complexes between calixarenes and aminesâ€™a reinvestigation. <i>Journal of Molecular Modeling</i> , 2006, 12, 739-747. | 0.8 | 21 |
| 2731 | Localized and delocalized perfluorosemibullvalenes. <i>Journal of Molecular Modeling</i> , 2006, 13, 133-136. | 0.8 | 2 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2732 | Heats of formation of GeH ₄ , GeF ₄ and Ge(CH ₃) ₄ . <i>Chemical Physics</i> , 2006, 324, 385-392. | 0.9 | 22 |
| 2733 | On the intramolecular proton transfer of 3-hydroxyflavone in the first singlet excited state: A theoretical study. <i>Chemical Physics</i> , 2006, 325, 243-250. | 0.9 | 38 |
| 2734 | Geometries and stabilities of 3d-transition metal-cation benzene complexes, M+Bzn (M=Scâ€“Cu, n=1, 2). <i>Chemical Physics</i> , 2006, 326, 600-604. | 0.9 | 30 |
| 2735 | Theoretical study of a neutral, doubly protonated, and doubly deprotonated porphyrin dithiolate used as a molecular switch. <i>Chemical Physics</i> , 2006, 327, 77-84. | 0.9 | 39 |
| 2736 | Trigonal bipyramidal iron(III) and manganese(III) oxo, sulfido, and selenido complexes. An electronic-structural overview. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 707-715. | 1.5 | 11 |
| 2737 | Syntheses, structures and electrochemistry of some 1-(1-allylamino)-1-ferrocenylcarbene complexes of chromium(0), molybdenum(0) and tungsten(0). <i>Journal of Organometallic Chemistry</i> , 2006, 691, 859-868. | 0.8 | 13 |
| 2738 | An experimental and theoretical investigation into the binding interactions of silver cluster cations with ethene and propene. <i>International Journal of Mass Spectrometry</i> , 2006, 249-250, 252-262. | 0.7 | 19 |
| 2739 | Investigations of the clustering reactions of protonated amino acid esters by high pressure mass spectrometry and quantum chemical calculations. <i>International Journal of Mass Spectrometry</i> , 2006, 255-256, 301-311. | 0.7 | 6 |
| 2740 | Elucidation of the absolute configuration of JNJ-27553292, a CCR2 receptor antagonist, by vibrational circular dichroism analysis of two precursors. <i>Chirality</i> , 2006, 18, 609-620. | 1.3 | 8 |
| 2741 | Computational Study of Solvent Effects and the Vibrational Spectra of Anderson Polyoxometalates. <i>Chemistry - A European Journal</i> , 2006, 12, 2094-2102. | 1.7 | 17 |
| 2742 | Gold(I)-Catalyzed Intramolecular Cyclopropanation of Dienes. <i>Chemistry - A European Journal</i> , 2006, 12, 1694-1702. | 1.7 | 163 |
| 2743 | The Characterisation of Molecular Alkali-Metal Azides. <i>Chemistry - A European Journal</i> , 2006, 12, 3580-3586. | 1.7 | 11 |
| 2744 | Tuning of Electronic Properties in Thienyl-Phosphole π -Conjugated Systems through P-Functionalization Monitored by Raman Spectroscopy. <i>Chemistry - A European Journal</i> , 2006, 12, 3759-3767. | 1.7 | 26 |
| 2745 | Optical, Redox, and NLO Properties of Tricyanovinyl Oligothiophenes: Comparisons between Symmetric and Asymmetric Substitution Patterns. <i>Chemistry - A European Journal</i> , 2006, 12, 5458-5470. | 1.7 | 37 |
| 2746 | Ethylene Biosynthesis by 1-Aminocyclopropane-1-Carboxylic Acid Oxidase: A DFT Study. <i>Chemistry - A European Journal</i> , 2006, 12, 8835-8846. | 1.7 | 40 |
| 2747 | Reactions of Th and U Atoms with C ₂ H ₂ : Infrared Spectra and Relativistic Calculations of the Metallacyclopentene, Actinide Insertion, and Ethynyl Products. <i>Chemistry - A European Journal</i> , 2006, 12, 8324-8335. | 1.7 | 37 |
| 2748 | Deconvoluting the Memory Effect in Pd-Catalyzed Allylic Alkylation: Effect of Leaving Group and Added Chloride. <i>Chemistry - A European Journal</i> , 2006, 12, 5352-5360. | 1.7 | 61 |
| 2749 | Local Aromaticity in Polycyclic Aromatic Hydrocarbons: Electron Delocalization versus Magnetic Indices. <i>Chemistry - A European Journal</i> , 2006, 12, 8813-8818. | 1.7 | 90 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2750 | The Importance of Inter- and Intramolecular van der Waals Interactions in Organic Reactions: the Dimerization of Anthracene Revisited. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 625-629. | 7.2 | 124 |
| 2751 | Designing Intermolecular Interactions between Halogenated Peripheries of Inorganic and Organic Molecules: Electrostatically Directed M _n X _n ...â€¦â€¦Xâ€²i _n C Halogen Bonds. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 435-440. | 7.2 | 152 |
| 2752 | Intrinsic Dinitrogen Activation at Bare Metal Atoms. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 6264-6288. | 7.2 | 117 |
| 2753 | Determination of the Relative Configuration of a Five-Membered Lactone from Residual Dipolar Couplings. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 4455-4460. | 7.2 | 80 |
| 2754 | 1,8-Bis(dimethylamino)naphthalene-2,7-diolate: A Simple Arylamine Nitrogen Base with Hydride-Ion-Comparable Proton Affinity. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 1453-1456. | 7.2 | 39 |
| 2755 | Experimental and Theoretical Characterization of Superoxide Complexes [W ₂ O ₆ (O ₂ ^{âˆ’})] and [W ₃ O ₉ (O ₂ ^{âˆ’})]: Models for the Interaction of O ₂ with Reduced W Sites on Tungsten Oxide Surfaces. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 657-660. | 7.2 | 66 |
| 2756 | Precedent and Theory Unite in the Hypothesis of a Highly Selective Fluoride Receptor. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 2890-2893. | 7.2 | 111 |
| 2757 | A Heterofulvene-Like Germylene with a Betain Reactivity. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 4349-4352. | 7.2 | 156 |
| 2758 | Seemingly Simple Stereoelectronic Effects in Alkane Isomers and the Implications for Kohnâ€™s Sham Density Functional Theory. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 4460-4464. | 7.2 | 360 |
| 2759 | Experimental Evidence for Linear Metalâ€™Azido Coordination: The Binary Group 5 Azides [Nb(N ₃) ₅], [Ta(N ₃) ₅], [Nb(N ₃) ₆] ^{âˆ’} , and [Ta(N ₃) ₆] ^{âˆ’} , and 1:1 Acetonitrile Adducts [Nb(N ₃) ₅ (CH ₃ CN)] and [Ta(N ₃) ₅ (CH ₃ CN)]. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 4830-4835. | 7.2 | 53 |
| 2760 | Proton Magnetic Shielding Tensors in Benzeneâ€™From the Individual Molecule to the Crystal. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 7292-7295. | 7.2 | 33 |
| 2761 | A Main-Group Analogue of Housene: The Subtle Influence of the Inert-Pair Effect in Group 15 Clusters. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 6685-6689. | 7.2 | 35 |
| 2762 | On the Usefulness of Bond Orders and Overlap Populations to Chalcogen-Nitrogen Systems. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 69-77. | 1.0 | 17 |
| 2763 | On the Existence of the Elusive Monomethyl Ester of Carbonic Acid [CH ₃ OC(O)OH] at 300 K: ¹ H- and ¹³ C NMR Measurements and DFT Calculations. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 908-913. | 1.0 | 48 |
| 2764 | Hydrogen Bonding and Proton Transfer to the Trihydride Complex [Cp*MoH ₃ (dppe)]: IR, NMR, and Theoretical Investigations. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 2192-2209. | 1.0 | 32 |
| 2765 | Quantum Chemical Analysis of the Enantiomerisation Mechanism of Complexes of the Type [M(III)(XU) ₄]F ⁺ (M = Pt, Pd, Ni; X = S, Se, Te; U = urea). <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 4063-4067. | 1.0 | 33 |
| 2766 | DFT Investigation of the Potential of [H-M{(NHCH ₂ CH ₂) ₃ X}] Catalysts (M = Mo, Ru, Os; X = N, P) for the Reduction of N ₂ to NH ₃ by H ₂ . <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 4407-4417. | 1.0 | 35 |
| 2767 | Chromogenic Meroterpenoids from the Mushrooms <i>Russula ochroleuca</i> and <i>R. viscida</i> . <i>European Journal of Organic Chemistry</i> , 2006, 2006, 1023-1033. | 1.2 | 52 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2768 | The Mechanism of Semibullvalene Bromination. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 738-745. | 1.2 | 7 |
| 2769 | Rearrangement of Electron-Rich N-Allyldibenzotetraazafulvalenes – An Experimental and Theoretical Study. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 3116-3124. | 1.2 | 34 |
| 2770 | A New Access to Chiral Phospholanes. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 3412-3420. | 1.2 | 17 |
| 2771 | Superacidic Activation of Maleimide and Phthalimide and Their Reactions with Cyclohexane and Arenes. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 4861-4866. | 1.2 | 29 |
| 2772 | Computation of vertical excitation energies of retinal and analogs: Scope and limitations. <i>Journal of Computational Chemistry</i> , 2006, 27, 116-123. | 1.5 | 25 |
| 2773 | Recognition of tandem sialic acid residues by CD38: A theoretical study. <i>Journal of Computational Chemistry</i> , 2006, 27, 53-60. | 1.5 | 2 |
| 2774 | A theoretical study of thermal [1,3]-sigmatropic rearrangements of 3-trimethylsilyl-1-pyrazoline: Concerted vs. stepwise mechanisms. <i>Journal of Computational Chemistry</i> , 2006, 27, 228-237. | 1.5 | 6 |
| 2775 | Activation barriers for DNA alkylation by carcinogenic methane diazonium ions. <i>Journal of Computational Chemistry</i> , 2006, 27, 277-286. | 1.5 | 30 |
| 2776 | Methane activation by chromium oxide cations in the gas phase: A theoretical study. <i>Journal of Computational Chemistry</i> , 2006, 27, 174-187. | 1.5 | 33 |
| 2777 | Starting SCF calculations by superposition of atomic densities. <i>Journal of Computational Chemistry</i> , 2006, 27, 926-932. | 1.5 | 57 |
| 2778 | Spin states in polynuclear clusters: The [Fe ₂ O ₂] core of the methane monooxygenase active site. <i>Journal of Computational Chemistry</i> , 2006, 27, 1223-1239. | 1.5 | 54 |
| 2779 | QM/MM calculations with DFT for taking into account protein effects on the EPR and optical spectra of metalloproteins. Plastocyanin as a case study. <i>Journal of Computational Chemistry</i> , 2006, 27, 1463-1475. | 1.5 | 107 |
| 2780 | Semiempirical GGA-type density functional constructed with a long-range dispersion correction. <i>Journal of Computational Chemistry</i> , 2006, 27, 1787-1799. | 1.5 | 24,222 |
| 2781 | Substituent Effect on Proton Affinity of Imidazole in Cu,Zn-Superoxide Dismutase. <i>Chinese Journal of Chemistry</i> , 2006, 24, 822-824. | 2.6 | 2 |
| 2782 | Synthesis and Structure-Activity Relationships of FAAH Inhibitors: Cyclohexylcarbamic Acid Biphenyl Esters with Chemical Modulation at the Proximal Phenyl Ring. <i>ChemMedChem</i> , 2006, 1, 130-139. | 1.6 | 59 |
| 2783 | Theoretical Analysis of the Terahertz Spectrum of the High Explosive PETN. <i>ChemPhysChem</i> , 2006, 7, 2398-2408. | 1.0 | 98 |
| 2784 | Eremophilane esters of <i>Robinsonia gerberifolia</i> and their rearranged products. Study of the coupling constants $^2J_{\text{H}}$, $^3J_{\text{H}}$, $^4J_{\text{H}}$. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, 30-34. | 1.1 | 3 |
| 2797 | Conceptual, Qualitative, and Quantitative Theories of 1,3-Dipolar and Diels-Alder Cycloadditions Used in Synthesis. <i>Advanced Synthesis and Catalysis</i> , 2006, 348, 2337-2361. | 2.1 | 273 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2798 | Quantum Chemical Investigations of Reaction Paths of Metalloenzymes and Biomimetic Models – The Hydrogenase Example. Topics in Current Chemistry, 2006, , 1-46. | 4.0 | 8 |
| 2799 | Application of Wigner and Husimi intracule based electron correlation models to excited states. Journal of Chemical Physics, 2006, 125, 074104. | 1.2 | 10 |
| 2800 | Calculation of two-photon absorption spectra of donor- π -acceptor compounds in solution using quadratic response time-dependent density functional theory. Journal of Chemical Physics, 2006, 125, 094103. | 1.2 | 63 |
| 2801 | The frequency-dependent dipole polarizability of the mercury dimer from four-component relativistic density-functional theory. Journal of Chemical Physics, 2006, 124, 044304. | 1.2 | 17 |
| 2802 | Structural implications of ring shape, dimension, and metal atom insertion in nanosized cyclic oligothiophenes: Joint Raman and density functional theory study. Journal of Chemical Physics, 2006, 125, 044518. | 1.2 | 12 |
| 2803 | Electronically excited states of tryptamine and its microhydrated complex. Journal of Chemical Physics, 2006, 125, 124309. | 1.2 | 27 |
| 2804 | Low frequency backbone vibrations of individual conformational isomers: Tryptamine. Journal of Chemical Physics, 2006, 125, 144303. | 1.2 | 17 |
| 2805 | Theoretical Study of Unsymmetrical Bisfullerene and Its Derivatives: C_{131} , C_{129BN} , and C_{130Si} . Journal of Physical Chemistry A, 2006, 110, 9921-9926. | 1.1 | 3 |
| 2806 | Accurate energies of hydrogen bonded nucleic acid base pairs and triplets in tRNA tertiary interactions. Nucleic Acids Research, 2006, 34, 865-879. | 6.5 | 79 |
| 2807 | Structural, electronic, and magnetic properties of FeSi: hybrid functionals and non-local exchange. Journal of Physics Condensed Matter, 2006, 18, 7437-7447. | 0.7 | 19 |
| 2808 | A restricted-open-shell complete-basis-set model chemistry. Journal of Chemical Physics, 2006, 125, 094106. | 1.2 | 208 |
| 2809 | Direct imaging of intracage structure in titanium-carbide endohedral metallofullerene. Physical Review B, 2006, 73, . | 1.1 | 35 |
| 2810 | A theoretical study of the chiroptical properties of molecules with isotopically engendered chirality. Journal of Chemical Physics, 2006, 124, 174301. | 1.2 | 52 |
| 2811 | Does the most stable formic acid tetramer have π stacking or $C\cdots H\cdots O$ interactions?. Journal of Chemical Physics, 2006, 124, 224313. | 1.2 | 20 |
| 2812 | Highly accurate ignition delay apparatus for hypergolic fuel research. Review of Scientific Instruments, 2006, 77, 045109. | 0.6 | 21 |
| 2813 | The electronic structure of oxo-Mn(salen): Single-reference and multireference approaches. Journal of Chemical Physics, 2006, 124, 144314. | 1.2 | 43 |
| 2814 | Effects of ionization on N-glycylglycine peptide: Influence of intramolecular hydrogen bonds. Journal of Chemical Physics, 2006, 124, 154306. | 1.2 | 26 |
| 2815 | Time-dependent density functional theory calculations for core-excited states: Assessment of standard exchange-correlation functionals and development of a novel hybrid functional. Journal of Chemical Physics, 2006, 124, 094105. | 1.2 | 73 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2816 | Cyclic Esters as Structural Fragments in Liquid Crystals. <i>Molecular Crystals and Liquid Crystals</i> , 2006, 457, 105-120. | 0.4 | 2 |
| 2817 | Energy gradients with respect to atomic positions and cell parameters for the Kohn-Sham density-functional theory at the Γ point. <i>Journal of Chemical Physics</i> , 2006, 124, 224107. | 1.2 | 2 |
| 2818 | Direct Experimental Probe of the On-Site Coulomb Repulsion in the Doubly Charged Fullerene Anion C_{70}^{2-} . <i>Physical Review Letters</i> , 2006, 96, 143002. | 2.9 | 71 |
| 2819 | Franck-Condon transitions in a system with large-amplitude anharmonic vibrations coupled to a harmonic-oscillator bath: Application to the C_{1s} photoelectron spectrum of ethanol. <i>Physical Review A</i> , 2006, 74, . | 1.0 | 9 |
| 2820 | Valence electronic structure of gas-phase 3,4,9,10-perylene tetracarboxylic acid dianhydride: Experiment and theory. <i>Physical Review B</i> , 2006, 73, . | 1.1 | 113 |
| 2821 | Ab-initiomolecular orbital theory of hydrogenation of $LiAl$ and Li_2Al_2 : The magic clusters $(LiAlH_4)$ and $(LiAlH_4)_2$. <i>Physical Review B</i> , 2006, 73, . | 1.1 | 5 |
| 2822 | Molecular quantum well at the C_{60} - $Au(111)$ interface. <i>Physical Review B</i> , 2006, 74, . | 1.1 | 26 |
| 2823 | From local hybrid functionals to σ -localized local hybrid potentials: Formalism and thermochemical tests. <i>Journal of Chemical Physics</i> , 2006, 124, 204102. | 1.2 | 64 |
| 2824 | A thermochemically competitive local hybrid functional without gradient corrections. <i>Journal of Chemical Physics</i> , 2007, 126, 011103. | 1.2 | 113 |
| 2825 | Theoretical study of the rhenium alkane interaction in transition metal alkane σ -complexes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 6963-6968. | 3.3 | 73 |
| 2826 | Computing Fukui functions without differentiating with respect to electron number. II. Calculation of condensed molecular Fukui functions. <i>Journal of Chemical Physics</i> , 2007, 126, 224108. | 1.2 | 58 |
| 2827 | Polynitrogen/Nanoaluminum Surface Interactions. , 2007, , . | | 0 |
| 2828 | Dimerization of (+)-Lysergic Acid Esters. <i>Heterocycles</i> , 2007, 71, 1075. | 0.4 | 4 |
| 2829 | Methodological aspects in the calculation of parity-violating effects in nuclear magnetic resonance parameters. <i>Journal of Chemical Physics</i> , 2007, 126, 074107. | 1.2 | 18 |
| 2830 | Gradients for two-component quasirelativistic methods. Application to dihalogenides of element 116. <i>Journal of Chemical Physics</i> , 2007, 126, 114106. | 1.2 | 25 |
| 2831 | Modeling the adiabatic connection in H_2 . <i>Journal of Chemical Physics</i> , 2007, 126, 244104. | 1.2 | 34 |
| 2832 | Electronic circular dichroism of disulphide bridge: Ab initio quantum-chemical calculations. <i>Journal of Chemical Physics</i> , 2007, 127, 085102. | 1.2 | 18 |
| 2833 | Xe_{129} chemical shift by the perturbational relativistic method: Xenon fluorides. <i>Journal of Chemical Physics</i> , 2007, 127, 084312. | 1.2 | 33 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2834 | Relativistic effects in the intermolecular interaction-induced nuclear magnetic resonance parameters of xenon dimer. <i>Journal of Chemical Physics</i> , 2007, 127, 164313. | 1.2 | 36 |
| 2835 | Unusual long-range spin-spin coupling in fluorinated polyenes: A mechanistic analysis. <i>Journal of Chemical Physics</i> , 2007, 127, 174704. | 1.2 | 10 |
| 2836 | Ab Initio potential grid based docking: From High Performance Computing to In Silico Screening. <i>AIP Conference Proceedings</i> , 2007, , . | 0.3 | 3 |
| 2837 | Chapter 4 Au _n and Ag _n (n=1-8) nanocluster catalysts: gas-phase reactivity to deposited structures. <i>Chemical Physics of Solid Surfaces</i> , 2007, , 151-199. | 0.3 | 16 |
| 2838 | Binding energies of hydrogen-bonded complexes from extrapolation with localized basis sets. <i>Journal of Chemical Physics</i> , 2007, 127, 085104. | 1.2 | 10 |
| 2839 | Transition metal NMR chemical shifts from optimized effective potentials. <i>Journal of Chemical Physics</i> , 2007, 126, 074101. | 1.2 | 22 |
| 2840 | Ab initio study of the torsional potential energy surfaces of N ₂ O ₃ and N ₂ O ₄ : Origin of the torsional barriers. <i>Journal of Chemical Physics</i> , 2007, 126, 154305. | 1.2 | 7 |
| 2841 | Assessment and formal properties of exchange-correlation functionals constructed from the adiabatic connection. <i>Journal of Chemical Physics</i> , 2007, 127, 034101. | 1.2 | 59 |
| 2842 | Range separated hybrid density functional with long-range Hartree-Fock exchange applied to solids. <i>Journal of Chemical Physics</i> , 2007, 127, 054101. | 1.2 | 89 |
| 2843 | Combining two-body density correlation functionals with multiconfigurational wave functions using natural orbitals and occupation numbers. <i>Journal of Chemical Physics</i> , 2007, 127, 104102. | 1.2 | 15 |
| 2844 | Theoretical predictions of nuclear magnetic resonance parameters in a novel organo-xenon species: Chemical shifts and nuclear quadrupole couplings in HXeCCH. <i>Journal of Chemical Physics</i> , 2007, 127, 234314. | 1.2 | 36 |
| 2845 | A Review of Density Functional Theory Quantum Mechanics as Applied to Pharmaceutically Relevant Systems. <i>Current Computer-Aided Drug Design</i> , 2007, 3, 290-296. | 0.8 | 28 |
| 2846 | Activation of C ₂ H ₆ and C ₃ H ₈ by Gas-Phase Mo ⁺ : Potential Energy Surfaces and Reaction Mechanisms. <i>Organometallics</i> , 2007, 26, 5486-5500. | 1.1 | 32 |
| 2847 | Dissociative electron attachment and electron energy-loss spectra of phenyl azide. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2007, 40, 101-109. | 0.6 | 14 |
| 2848 | Theoretical Study on the Electronic and Electrical Properties of p-Type Transparent Conducting Metal Oxides. <i>Japanese Journal of Applied Physics</i> , 2007, 46, 2603-2608. | 0.8 | 2 |
| 2849 | Density functional calculations of NMR shielding tensors for paramagnetic systems with arbitrary spin multiplicity: Validation on 3d metallocenes. <i>Journal of Chemical Physics</i> , 2007, 126, 024107. | 1.2 | 98 |
| 2850 | Combining multiconfigurational wave functions with correlation density functionals: A size-consistent method based on natural orbitals and occupation numbers. <i>Physical Review A</i> , 2007, 75, . | 1.0 | 37 |
| 2851 | Theoretical investigation of silicon nanowires: Methodology, geometry, surface modification, and electrical conductivity using a multiscale approach. <i>Physical Review B</i> , 2007, 76, . | 1.1 | 102 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2852 | Nuclear magnetic resonance parameters of atomic xenon dissolved in Gay-Berne model liquid crystal. <i>Physical Review E</i> , 2007, 75, 031707. | 0.8 | 11 |
| 2853 | Factors affecting imine coordination in (iminoterpyridine)MX ₂ (M = Fe, Co, Ni, Zn): synthesis, structures, DFT calculations and ethylene oligomerisation studies. <i>New Journal of Chemistry</i> , 2007, 31, 75-85. | 1.4 | 30 |
| 2854 | Density functional study of the interaction between small Au clusters, Au _n (n=1-7) and the rutile TiO ₂ surface. II. Adsorption on a partially reduced surface. <i>Journal of Chemical Physics</i> , 2007, 127, 244708. | 1.2 | 52 |
| 2855 | Current-voltage curves for molecular junctions: Effect of substituents. <i>Physical Review B</i> , 2007, 75, . | 1.1 | 20 |
| 2856 | Density functional study of the electronic and vibrational properties of TiOCl. <i>Physical Review B</i> , 2007, 76, . | 1.1 | 10 |
| 2857 | Structural properties and magic structures in hydrogenated finite and infinite silicon nanowires. <i>Applied Physics Letters</i> , 2007, 91, 203112. | 1.5 | 16 |
| 2858 | The importance of middle-range Hartree-Fock-type exchange for hybrid density functionals. <i>Journal of Chemical Physics</i> , 2007, 127, 221103. | 1.2 | 152 |
| 2859 | Insights into Cu(I) Exchange in HAH1 Using Quantum Mechanical and Molecular Simulations. <i>Biochemistry</i> , 2007, 46, 8816-8826. | 1.2 | 52 |
| 2860 | Optimization of quantum Monte Carlo wave functions by energy minimization. <i>Journal of Chemical Physics</i> , 2007, 126, 084102. | 1.2 | 226 |
| 2861 | Ab-initio thermal physics and Cr-isotopic fractionation of MgCr ₂ O ₄ . <i>American Mineralogist</i> , 2007, 92, 98-108. | 0.9 | 8 |
| 2862 | Characterization of Copper(II) Interactions with Sinefungin, a Nucleoside Antibiotic: Combined Potentiometric, Spectroscopic and DFT Studies. <i>Bioinorganic Chemistry and Applications</i> , 2007, 2007, 1-12. | 1.8 | 1 |
| 2863 | Local hybrid functionals based on density matrix products. <i>Journal of Chemical Physics</i> , 2007, 127, 164117. | 1.2 | 54 |
| 2864 | Application of Bond Energy Density Analysis (Bond-EDA) to Diels-Alder Reaction. <i>Chemistry Letters</i> , 2007, 36, 616-617. | 0.7 | 10 |
| 2865 | Theoretical Design of Monofunctional Psoralen Compounds in Photochemotherapy. <i>Bulletin of the Chemical Society of Japan</i> , 2007, 80, 1341-1349. | 2.0 | 5 |
| 2866 | Theoretical Study of Geometries and Electronic Transition of Color-Switching Molecules: Tetra-Aza Macrocyclic and Its Zinc Complexes. <i>Bulletin of the Chemical Society of Japan</i> , 2007, 80, 686-693. | 2.0 | 4 |
| 2867 | Quantum Mechanics for Organic Chemistry. , 0, , 1-41. | | 1 |
| 2868 | The Energetics for Hydrogen Addition to Naphthalene Cations. <i>Astrophysical Journal</i> , 2007, 659, 858-861. | 1.6 | 15 |
| 2869 | Tetrathiafulvalene-Based Materials for Organic Field Effect Transistors. Inspection of Their Semiconductor Properties by Means of Molecular Spectroscopy and Quantum Chemistry. <i>Journal of Physical Chemistry C</i> , 2007, 111, 10110-10118. | 1.5 | 20 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2870 | Electronic and Vibrational Spectroscopy of Diamondoids and the Interstellar Infrared Bands between 3.35 and 3.55 μm . <i>Astrophysical Journal</i> , 2007, 671, 458-469. | 1.6 | 47 |
| 2871 | DFT Studies on the Mechanism of Reactions between N ₂ O and Cp ₂ M(η -2-alkyne) (M = Ti, Zr). <i>Organometallics</i> , 2007, 26, 6769-6777. | 1.1 | 17 |
| 2872 | A Missing Reaction Step in Dithiobenzoate-Mediated RAFT Polymerization. <i>Macromolecular Symposia</i> , 2007, 248, 158-167. | 0.4 | 25 |
| 2873 | Hydrogen Transfer to Ketones Catalyzed by Shvo's Ruthenium Hydride Complex: A Mechanistic Insight. <i>Organometallics</i> , 2007, 26, 4135-4144. | 1.1 | 130 |
| 2874 | Long-Distance Structural Consequences of H-Bonding. How H-Bonding Affects Aromaticity of the Ring in Variously Substituted Aniline/Anilinium/Anilide Complexes with Bases and Acids. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 875-886. | 2.5 | 30 |
| 2875 | Comparison of DFT Methods for Molecular Orbital Eigenvalue Calculations. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1554-1561. | 1.1 | 693 |
| 2876 | BFW: A Density Functional for Transition Metal Clusters. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2625-2628. | 1.1 | 8 |
| 2877 | Theoretical study of corrosion inhibition of amides and thiosemicarbazones. <i>Corrosion Science</i> , 2007, 49, 2118-2130. | 3.0 | 180 |
| 2878 | Finite-Length Models of Carbon Nanotubes Based on Clar Sextet Theory. <i>Organic Letters</i> , 2007, 9, 4267-4270. | 2.4 | 53 |
| 2879 | Influence of π -Conjugation Units in Organic Dyes for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1853-1860. | 1.5 | 160 |
| 2880 | Infrared Spectrum and Bonding in Uranium Methylidene Dihydride, CH ₂ UH ₂ . <i>Inorganic Chemistry</i> , 2007, 46, 4917-4925. | 1.9 | 73 |
| 2881 | Self-Consistent Reaction Field Model for Aqueous and Nonaqueous Solutions Based on Accurate Polarized Partial Charges. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2011-2033. | 2.3 | 426 |
| 2882 | Structural Analysis of the Anti-Malaria Active Agent Chloroquine under Physiological Conditions. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1815-1822. | 1.2 | 46 |
| 2883 | Assessment of long-range corrected functionals performance for $n\pi^*$ transitions in organic dyes. <i>Journal of Chemical Physics</i> , 2007, 127, 094102. | 1.2 | 119 |
| 2884 | Critical Assessment of the Performance of Density Functional Methods for Several Atomic and Molecular Properties. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 407-433. | 2.3 | 295 |
| 2885 | Aqueous Microsolvation of Mercury Halide Species. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11342-11349. | 1.1 | 28 |
| 2886 | On the position of the potential wall in DFT temporary anion calculations. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5880. | 1.3 | 33 |
| 2887 | From Azobenzene Coordination to Aryl-Halide Bond Activation by Platinum. <i>Organometallics</i> , 2007, 26, 4528-4534. | 1.1 | 39 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2888 | Water Exchange on Seven-Coordinate Mn(II) Complexes with Macrocyclic Pentadentate Ligands: Insight in the Mechanism of Mn(II) SOD Mimetics. <i>Inorganic Chemistry</i> , 2007, 46, 2459-2470. | 1.9 | 95 |
| 2889 | First-Principles Calculation of ρ_{K} for Cocaine, Nicotine, Neurotransmitters, and Anilines in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2007, 111, 10599-10605. | 1.2 | 71 |
| 2890 | A Class of Luminescent Cyclometalated Alkynylgold(III) Complexes: Synthesis, Characterization, and Electrochemical, Photophysical, and Computational Studies of $[\text{Au}(\text{C}_6\text{N}_3\text{SC})(\text{C}_6\text{CR})]$ ($\text{C}_6\text{N}_3\text{SC} = \text{1}^3\text{C,N,C}$) Tj^{BTQO} $\text{O}^{\text{BT/Ove}}$ | 1.7 | 108 |
| 2891 | Linear and Nonlinear Optical Properties of Pyridine-Based Octopolar Chromophores Designed for Chemical Sensing. Joint Spectroscopic and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 18778-18784. | 1.5 | 25 |
| 2892 | Double-hybrid density functional theory for excited electronic states of molecules. <i>Journal of Chemical Physics</i> , 2007, 127, 154116. | 1.2 | 404 |
| 2893 | Assessment of the exchange-correlation functionals for the physical description of spin transition phenomena by density functional theory methods: All the same?. <i>Journal of Chemical Physics</i> , 2007, 126, 014105. | 1.2 | 102 |
| 2894 | Thiophene- and Selenophene-Based Heteroacenes: Combined Quantum Chemical DFT and Spectroscopic Raman and UV-Vis-NIR Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 7488-7496. | 1.2 | 32 |
| 2895 | Density functional theory with dispersion corrections for supramolecular structures, aggregates, and complexes of (bio)organic molecules. <i>Organic and Biomolecular Chemistry</i> , 2007, 5, 741-758. | 1.5 | 683 |
| 2896 | Charge Transport in Conjugated Aromatic Molecular Junctions: Molecular Conjugation and Molecule-Electrode Coupling. <i>Journal of Physical Chemistry C</i> , 2007, 111, 14893-14902. | 1.5 | 91 |
| 2897 | Meta-generalized gradient approximation: non-empirical construction and performance of a density functional. <i>Philosophical Magazine</i> , 2007, 87, 1071-1084. | 0.7 | 11 |
| 2898 | How Well Can New-Generation Density Functionals Describe Protonated Epoxides Where Older Functionals Fail?. <i>Journal of Organic Chemistry</i> , 2007, 72, 295-298. | 1.7 | 41 |
| 2899 | Choline Saccharinate and Choline Acesulfamate: Ionic Liquids with Low Toxicities. <i>Journal of Physical Chemistry B</i> , 2007, 111, 5254-5263. | 1.2 | 224 |
| 2900 | H ₂ O ₃ as a Reactive Oxygen Species: Formation of 8-Oxoguanine from Its Reaction with Guanine. <i>Journal of Physical Chemistry B</i> , 2007, 111, 4603-4615. | 1.2 | 25 |
| 2901 | Calculations on Open-Shell Molecules: A Beginner's Guide. <i>Reviews in Computational Chemistry</i> , 2007, 1-97. | 1.5 | 77 |
| 2902 | Structure and bonding in boron carbide: The invincibility of imperfections. <i>New Journal of Chemistry</i> , 2007, 31, 473. | 1.4 | 118 |
| 2903 | Density Functional Theory Treatment of Electron Correlation in the Nuclear-Electronic Orbital Approach. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4522-4526. | 1.1 | 74 |
| 2904 | General Transition-State Force Field for Cytochrome P450 Hydroxylation. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1765-1773. | 2.3 | 54 |
| 2905 | Highly Selective Diels-Alder Reactions of Directly Connected Enyne Dienophiles. <i>Journal of the American Chemical Society</i> , 2007, 129, 645-657. | 6.6 | 45 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2906 | Influence of the Side Chain in the Structure and Fragmentation of Amino Acids Radical Cations. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2210-2220. | 2.3 | 41 |
| 2907 | Coordinatively Unsaturated Semisandwich Complexes of Ruthenium with Phosphinoamine Ligands and Related Species: A Complex Containing (R)-1,2-Bis((diisopropylphosphino)amino)cyclohexane in a New Coordination Form $P^3</math>-N</math>. Inorganic Chemistry, 2007, 46, 6958-6967.$ | 1.9 | 34 |
| 2908 | A Detailed Theoretical Study of the Mechanism and Energetics of Methane to Methanol Conversion by Cisplatin and Catalytic. <i>Organometallics</i> , 2007, 26, 793-809. | 1.1 | 49 |
| 2909 | Thermochemistry and Infrared Spectroscopy of Neutral and Cationic Iron Polycyclic Aromatic Hydrocarbon Complexes of Astrophysical Interest: A Fundamental Density Functional Theory Studies. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9745-9755. | 1.1 | 38 |
| 2910 | Spin-Polarized Conceptual Density Functional Theory Study of the Regioselectivity in Ring Closures of Radicals. <i>Journal of Organic Chemistry</i> , 2007, 72, 348-356. | 1.7 | 36 |
| 2911 | Spin-State Energetics and Spin-Crossover Behavior of Pseudotetrahedral Cobalt(III) Imido Complexes. The Role of the Tripodal Supporting Ligand. <i>Inorganic Chemistry</i> , 2007, 46, 7890-7898. | 1.9 | 51 |
| 2912 | Polarizability and second hyperpolarizability evaluation of long molecules by the density functional theory with long-range correction. <i>Journal of Chemical Physics</i> , 2007, 126, 014107. | 1.2 | 190 |
| 2913 | On the definition of local spin in relativistic and nonrelativistic quantum chemistry. <i>Faraday Discussions</i> , 2007, 135, 97-124. | 1.6 | 68 |
| 2914 | Mechanism of Formation of Silver Heterocyclic Carbenes Using Silver Oxide: A Theoretical Study. <i>Organometallics</i> , 2007, 26, 6170-6183. | 1.1 | 58 |
| 2915 | The Adsorption of Perfluorooctane Sulfonate onto Sand, Clay, and Iron Oxide Surfaces. <i>Journal of Chemical & Engineering Data</i> , 2007, 52, 1165-1170. | 1.0 | 290 |
| 2916 | Pseudohelical and Helical Primary Structures of 1,2-Spiroannulated Four- and Five-Membered Rings: Syntheses and Chiroptical Properties. <i>Journal of Organic Chemistry</i> , 2007, 72, 9264-9277. | 1.7 | 18 |
| 2917 | Attractive Noncovalent Interactions in the Mechanism of Grubbs Second-Generation Ru Catalysts for Olefin Metathesis. <i>Organic Letters</i> , 2007, 9, 1967-1970. | 2.4 | 163 |
| 2918 | Analysis of Nuclear Quantum Effects on Hydrogen Bonding. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2206-2212. | 1.1 | 38 |
| 2919 | Density Functional Theory Methods as Powerful Tools to Elucidate Amino Acid Oxidation Mechanisms. A Case Study on Methionine Model Peptide. <i>Journal of Physical Chemistry B</i> , 2007, 111, 485-489. | 1.2 | 14 |
| 2920 | Oxidation of Tertiary Silanes by Osmium Tetroxide. <i>Inorganic Chemistry</i> , 2007, 46, 5212-5219. | 1.9 | 73 |
| 2921 | Dissecting the Proline Effect: Dissociations of Proline Radicals Formed by Electron Transfer to Protonated Pro-Gly and Gly-Pro Dipeptides in the Gas Phase. <i>Journal of the American Chemical Society</i> , 2007, 129, 7936-7949. | 6.6 | 50 |
| 2922 | Aromaticity and Curvature in Heteroacepentalenes. <i>Journal of Organic Chemistry</i> , 2007, 72, 4323-4327. | 1.7 | 22 |
| 2923 | Computational Studies of Radicals Relevant to Nucleic Acid Damage. <i>Advances in Quantum Chemistry</i> , 2007, 52, 89-120. | 0.4 | 20 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2924 | Analytic derivatives for perturbatively corrected $\hat{\rho}$ -double hybrid density functionals: Theory, implementation, and applications. <i>Journal of Chemical Physics</i> , 2007, 126, 124115. | 1.2 | 173 |
| 2925 | Density Functional Theory and Atoms-in-Molecules Investigation of Intramolecular Hydrogen Bonding in Derivatives of Malonaldehyde and Implications for Resonance-Assisted Hydrogen Bonding. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8519-8530. | 1.1 | 109 |
| 2926 | Water-Assisted H $\hat{\nu}$ -H Bond Splitting Mediated by [CpRu(PTA)2Cl] (PTA=1,3,5-triaza-7-phosphaadamantane). A DFT Analysis. <i>Organometallics</i> , 2007, 26, 3289-3296. | 1.1 | 57 |
| 2927 | Vibronic Interaction in Metalloporphyrin $\hat{\nu}$ -Anion Radicals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 852-857. | 1.1 | 12 |
| 2928 | Mechanistic Studies on the Stereoselective Formation of $\hat{\nu}$ -Mannosides from Mannosyl Iodides Using $\hat{\nu}$ -Deuterium Kinetic Isotope Effects. <i>Journal of Organic Chemistry</i> , 2007, 72, 4663-4672. | 1.7 | 58 |
| 2929 | On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters: Benchmarks approaching the complete basis set limit. <i>Journal of Chemical Physics</i> , 2007, 127, 184104. | 1.2 | 208 |
| 2930 | Electroweak interactions in chiral molecules: two-component density functional theory study of vibrational frequency shifts in polyhalomethanes. <i>Molecular Physics</i> , 2007, 105, 41-49. | 0.8 | 30 |
| 2931 | The spin coupling in the diiron complex [Fe ₂ (hpdta)(H ₂ O) ₃ Cl]. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 1911-1920. | 1.3 | 13 |
| 2932 | Density Functional Study of Lithium Hexamethyldisilazide (LiHMDS) Complexes: $\hat{\nu}$ Effects of Solvation and Aggregation. <i>Inorganic Chemistry</i> , 2007, 46, 3856-3864. | 1.9 | 17 |
| 2933 | Anharmonic Effects in Ammonium Nitrate and Hydroxylammonium Nitrate Clusters. <i>Journal of Physical Chemistry B</i> , 2007, 111, 4653-4658. | 1.2 | 19 |
| 2934 | H $\hat{\nu}$ -ZSM-5 Modified Zeolite: $\hat{\nu}$ Quantum Chemical Models of Acidic Sites. <i>Journal of Physical Chemistry C</i> , 2007, 111, 13033-13043. | 1.5 | 36 |
| 2935 | Electron Super-Rich Radicals in the Gas Phase. A Neutralization- $\hat{\nu}$ Reionization Mass Spectrometric and ab Initio/RRKM Study of Diaminohydroxymethyl and Triaminomethyl Radicals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8829-8843. | 1.1 | 19 |
| 2936 | Geometric Structure of X(AuPH ₃) ₄ ⁺ (X = N, P, As, Sb): $\hat{\nu}$ Td or C _{4v} ?. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1562-1566. | 1.1 | 15 |
| 2937 | Theoretical Elucidation of the Platinum-Mediated Arene C $\hat{\nu}$ -H Activation Reactions. <i>Organometallics</i> , 2007, 26, 2203-2210. | 1.1 | 16 |
| 2938 | Intersystem crossing driven by vibronic spin-orbit coupling: a case study on psoralen. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5209. | 1.3 | 129 |
| 2939 | A tautomeric equilibrium between functionalized 2-formylphenylboronic acids and corresponding 1,3-dihydro-1,3-dihydroxybenzo[c][2,1]oxaboroles. <i>New Journal of Chemistry</i> , 2007, 31, 144-154. | 1.4 | 51 |
| 2940 | Reaction and subsequent transformation of anionic acetylide-carbene complexes using the Ph ₃ PAu ⁺ fragment. <i>Dalton Transactions</i> , 2007, , 5684. | 1.6 | 9 |
| 2941 | Correlated proton motion in hydrogen bonded systems: tuning proton affinities. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 299-310. | 1.3 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 2942 | Molecular recognition in molecular tweezers systems: quantum-chemical calculation of NMR chemical shifts. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 4552. | 1.3 | 21 |
| 2943 | Spectroscopic properties of trichlorofluoromethane CCl ₃ F calculated by density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5027. | 1.3 | 2 |
| 2944 | Feasibility of associative mechanism in enyne metathesis catalyzed by grubbs complexes. <i>Dalton Transactions</i> , 2007, , 2925-2934. | 1.6 | 13 |
| 2945 | Electrochemical and theoretical investigations of the reduction of [Fe ₂ (CO) ₅ L{μ-SCH ₂ XCH ₂ S}] complexes related to [FeFe] hydrogenase. <i>New Journal of Chemistry</i> , 2007, 31, 2052. | 1.4 | 98 |
| 2946 | Pairing strength and proton characters of the N7,N9-dimethylated GC and AT base pairs: a density functional theory investigation. <i>New Journal of Chemistry</i> , 2007, 31, 1514. | 1.4 | 4 |
| 2947 | Optical Properties of the Phosphorescent Trinuclear Copper(I) Complexes of Pyrazolates: Insights from Theory. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4965-4973. | 1.1 | 42 |
| 2948 | Time-Dependent Density Functional Theory Study of the X-ray Absorption Spectroscopy of Acetylene, Ethylene, and Benzene on Si(100). <i>Journal of Physical Chemistry C</i> , 2007, 111, 3333-3340. | 1.5 | 76 |
| 2949 | Analysis of Conformer Stability for 1,3,8-Trihydroxynaphthalene: A Natural Substrate of Fungal Trihydroxynaphthalene Reductase. <i>Journal of Physical Chemistry B</i> , 2007, 111, 8314-8320. | 1.2 | 2 |
| 2950 | ¹² -Hydrogen Kinetic Effect. <i>Journal of the American Chemical Society</i> , 2007, 129, 5744-5755. | 6.6 | 29 |
| 2951 | Accurate Description of Nitrogenous Base Flexibility in Classical Molecular Dynamics Simulations of Nucleotides Bound to Proteins. <i>Journal of Physical Chemistry B</i> , 2007, 111, 6297-6302. | 1.2 | 6 |
| 2952 | Ultrasensitive in situ Tracing of the Alkaloid Dioncophylline A in the Tropical Liana <i>Triphyophyllum peltatum</i> by Applying Deep-UV Resonance Raman Microscopy. <i>Analytical Chemistry</i> , 2007, 79, 986-993. | 3.2 | 46 |
| 2953 | Electrostatically Embedded Many-Body Expansion for Large Systems, with Applications to Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 46-53. | 2.3 | 254 |
| 2954 | Platinum Group Thiophenoxyimine Complexes: Syntheses and Crystallographic/Computational Studies. <i>Organometallics</i> , 2007, 26, 897-909. | 1.1 | 22 |
| 2955 | Dipole Formation at Interfaces of Alkanethiolate Self-assembled Monolayers and Ag(111). <i>Journal of Physical Chemistry C</i> , 2007, 111, 14448-14456. | 1.5 | 55 |
| 2956 | DFT Studies of ¹² -Boryl Elimination Processes: Potential Role in Catalyzed Borylation Reactions of Alkenes. <i>Organometallics</i> , 2007, 26, 3149-3156. | 1.1 | 40 |
| 2957 | Effect of Ring Strain on Nucleophilic Substitution at Selenium: A Computational Study of Cyclic Diselenides and Selenenyl Sulfides. <i>Journal of Organic Chemistry</i> , 2007, 72, 5174-5182. | 1.7 | 31 |
| 2958 | Oriental Order Properties in Fluorinated Liquid Crystals from an Optical, Dielectric, and ¹³ C NMR Combined Approach. <i>Journal of Physical Chemistry C</i> , 2007, 111, 5286-5299. | 1.5 | 24 |
| 2959 | A Density Functional Theory Study of the Electronic Properties of Os(II) and Os(III) Complexes Immobilized on Au(111). <i>Inorganic Chemistry</i> , 2007, 46, 117-124. | 1.9 | 12 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2960 | Theoretical Prediction of the p53 Gene Mutagenic Mechanism Induced by trans-4-Hydroxy-2-nonenal. <i>Journal of Physical Chemistry B</i> , 2007, 111, 5362-5371. | 1.2 | 10 |
| 2961 | Electronic and Molecular Structures of Trigonal Truxene-Core Systems Conjugated to Peripheral Fluorene Branches. Spectroscopic and Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 4026-4035. | 1.2 | 36 |
| 2962 | Comparative Assessment of Theoretical Methods for the Determination of Geometrical Properties in Biological Zinc Complexes. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9146-9152. | 1.2 | 32 |
| 2963 | Ab Initio Energies and Product Branching Ratios for the O + C ₃ H ₆ Reaction. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12977-12984. | 1.1 | 12 |
| 2964 | DFT Study of Hydride Exchange in a Binuclear Ruthenium Complex. <i>Organometallics</i> , 2007, 26, 56-64. | 1.1 | 11 |
| 2965 | Electron Transfer to Protonated $\hat{\text{I}}^2$ -Alanine N-Methylamide in the Gas Phase: An Experimental and Computational Study of Dissociation Energetics and Mechanisms. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4167-4180. | 1.1 | 19 |
| 2966 | Determining the Structure of Silica-Supported Monomeric Vanadium Oxide Catalysts Based on Synthesis Method and Spectral Data from Theoretical Calculations. <i>Journal of Physical Chemistry C</i> , 2007, 111, 7071-7077. | 1.5 | 12 |
| 2967 | Ab Initio, Density Functional Theory, and Continuum Solvation Model Prediction of the Product Ratio in the S _N 2 Reaction of NO ₂ with CH ₃ CH ₂ Cl and CH ₃ CH ₂ Br in DMSO Solution. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10068-10074. | 1.1 | 21 |
| 2968 | On the Copper(II) Ion Coordination by Prion Protein HGGGW Pentapeptide Model. <i>Journal of Physical Chemistry B</i> , 2007, 111, 635-640. | 1.2 | 34 |
| 2969 | Perturbing the Structure of the 2-Norbornyl Cation through C $\hat{\text{a}}^{\sim}$ H $\hat{\text{A}}^{\sim}$ $\hat{\text{A}}^{\sim}$ N and C $\hat{\text{a}}^{\sim}$ H $\hat{\text{A}}^{\sim}$ $\hat{\text{A}}^{\sim}$ I $\hat{\text{E}}$ Interactions. <i>Journal of Organic Chemistry</i> , 2007, 72, 8877-8881. | 1.7 | 50 |
| 2970 | N,N-Di(4-halophenyl)nitrenium Ions: A Nucleophilic Trapping, Aromatic Substitution, and Hydrogen Atom Transfer. <i>Journal of Organic Chemistry</i> , 2007, 72, 4626-4634. | 1.7 | 16 |
| 2971 | Substituent Effects on the Structures of Silver Complexes with Monoaza-trithia-12-Crown-4 Ethers Bearing Substituted Aromatic Rings. <i>Inorganic Chemistry</i> , 2007, 46, 6529-6534. | 1.9 | 22 |
| 2972 | Theoretical Study of the Reaction Mechanisms Involved in the Thermal Intramolecular Reactions of 1,6-Fullerenynes. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5253-5258. | 1.1 | 12 |
| 2973 | Computational Studies of Intramolecular Hydrogen Atom Transfers in the $\hat{\text{I}}^2$ -Hydroxyethylperoxy and $\hat{\text{I}}^2$ -Hydroxyethoxy Radicals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5032-5042. | 1.1 | 37 |
| 2974 | Aromaticity of Distorted Benzene Rings: Exploring the Validity of Different Indicators of Aromaticity. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4513-4521. | 1.1 | 102 |
| 2975 | Scaled Density Functional Theory Correlation Functionals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10390-10399. | 1.1 | 0 |
| 2976 | Polarizability of Small Carbon Cluster Anions from First Principles. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2028-2032. | 1.1 | 15 |
| 2977 | A Density Functional Study of the Various Forms of UN ₄ O ₁₂ Containing Uranyl Nitrate. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10789-10803. | 1.1 | 8 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 2978 | Density Functional Study of EPR Parameters and Spin-Density Distribution of Azurin and Other Blue Copper Proteins. <i>Journal of Physical Chemistry B</i> , 2007, 111, 8290-8304. | 1.2 | 63 |
| 2979 | The Reaction of <i>n</i> - and <i>i</i> -C ₄ H ₉ Radicals with Acetylene. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3740-3747. | 1.1 | 83 |
| 2980 | Substituent Effects on Tandem Alkenyl Migration/Electrophilic Aromatic Substitution Reactions: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2007, 72, 8394-8401. | 1.7 | 9 |
| 2981 | Mechanistic Aspects of the Formation of Aldehydes and Nitriles in Photosensitized Reactions of Aldoxime Ethers. <i>Journal of Organic Chemistry</i> , 2007, 72, 4126-4134. | 1.7 | 12 |
| 2982 | Factors Determining the Driving Force of DNA Formation: Geometrical Differences of Base Pairs, Dehydration of Bases, and the Arginine Assisting. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1802-1808. | 1.2 | 4 |
| 2983 | Polymeric Alkylidene-Bridged Platinum Complex $[\{Pt_2(\eta^4-CI)2(\eta^4-C(OBu)Me)2\}_n]$: Synthesis, Reactivity, and Quantum Chemical Calculations. <i>Organometallics</i> , 2007, 26, 6000-6008. | 1.1 | 2 |
| 2984 | Crucial Role of Anions on the Deprotonation of the Cationic Dihydrogen Complex $trans-[FeH(\eta^2-H_2)(dppe)_2]^+$. <i>Journal of the American Chemical Society</i> , 2007, 129, 6608-6618. | 6.6 | 51 |
| 2985 | Surface-Enhanced Raman Spectroscopy of Soft-Landed Polyatomic Ions and Molecules. <i>Analytical Chemistry</i> , 2007, 79, 4543-4551. | 3.2 | 64 |
| 2986 | Tunable π -Interactions in Monomeric Organozinc Complexes: Solution and Solid-State Studies. <i>Organometallics</i> , 2007, 26, 4015-4020. | 1.1 | 30 |
| 2987 | Molecular Electronics with Endohedral Metallofullerenes: The Test Case of $La_{2@C_{80}}$ Nanjunctions. <i>Journal of Physical Chemistry C</i> , 2007, 111, 17640-17645. | 1.5 | 21 |
| 2988 | Intramolecular Rearrangement of Organosilyl Groups in Silylamines: A Combined Experimental/Theoretical Study. <i>Organometallics</i> , 2007, 26, 838-845. | 1.1 | 9 |
| 2989 | The Ultrafast Dynamics of Hydrogen-Bonded Liquids: Molecular Structure-Dependent Occurrence of Normal Arrhenius or Fractional Stokes-Einstein-Debye Rotational Diffusive Relaxation. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9634-9643. | 1.2 | 22 |
| 2990 | Mechanism of Photoinduced Decomposition of Ketoprofen. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 1735-1743. | 2.9 | 69 |
| 2991 | Characterization of the Tyrosine-Z Radical and Its Environment in the Spin-Coupled S ₂ TyrZ State of Photosystem II from <i>Thermosynechococcus elongatus</i> . <i>Biochemistry</i> , 2007, 46, 3138-3150. | 1.2 | 35 |
| 2992 | An Experimental and Theoretical Study of the Asymmetric Lithiation of 1,2,3,5,6,7-Hexahydro-3a,4a-diazacyclopenta[def]phenanthren-4-one. <i>Journal of Organic Chemistry</i> , 2007, 72, 957-963. | 1.7 | 12 |
| 2993 | Nature of Cp*MoO ₂ ⁺ in Water and Intramolecular Proton-Transfer Mechanism by Stopped-Flow Kinetics and Density Functional Theory Calculations. <i>Inorganic Chemistry</i> , 2007, 46, 4103-4113. | 1.9 | 39 |
| 2994 | Origin of the Anomalous Two-Photon Absorption in Fluorescent Protein DsRed. <i>Journal of Physical Chemistry B</i> , 2007, 111, 505-507. | 1.2 | 24 |
| 2995 | DFT Calculations on [6.8]Cyclacenes and CpCo-Capped [4.8]Cyclacenes. <i>Organic Letters</i> , 2007, 9, 4037-4040. | 2.4 | 24 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 2996 | A Computational Study on the Interaction of the Nitric Oxide Ions NO ⁺ and NO ⁻ with the Side Groups of the Aromatic Amino Acids. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1981-1989. | 1.1 | 13 |
| 2997 | Chromophore Localization in Conjugated Polymers: Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , 2007, 111, 12053-12058. | 1.2 | 13 |
| 2998 | Predictions of Novel Two-Photon Absorption Bands in Fluorescent Proteins. <i>Journal of Physical Chemistry B</i> , 2007, 111, 14043-14050. | 1.2 | 46 |
| 2999 | Organotin(IV) Derivatives of Some O,C,O-Chelating Ligands. Part 2. <i>Organometallics</i> , 2007, 26, 6312-6319. | 1.1 | 17 |
| 3000 | Spectroscopic and Density Functional Theory Studies of the Molecular Geometry and Electronic Structure of Classical and Nonclassical Radical Ions Derived from 7-Benzhydrylidenebornene Analogues. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7898-7905. | 1.1 | 7 |
| 3001 | A QM/MM Study of the Bergman Reaction of Dynemicin A in the Minor Groove of DNA. <i>Journal of Physical Chemistry B</i> , 2007, 111, 8321-8328. | 1.2 | 16 |
| 3002 | chapter 2 Obtaining Molecular Thermochemistry from Calculations. <i>Comprehensive Chemical Kinetics</i> , 2007, , 7-42. | 2.3 | 2 |
| 3003 | Experimental and Computational Studies of the Phenyl Radical Reaction with Allene. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6881-6889. | 1.1 | 17 |
| 3004 | Ab Initio Thermochemistry of the Hydrogenation of Hydrocarbon Radicals Using Silicon-, Germanium-, Tin-, and Lead-Substituted Methane and Isobutane. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8677-8688. | 1.1 | 12 |
| 3005 | Successful a Priori Modeling of CO Adsorption on Pt(111) Using Periodic Hybrid Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2007, 129, 10402-10407. | 6.6 | 73 |
| 3006 | Organocatalytic Claisen Rearrangement: Theory and Experiment. <i>Journal of Organic Chemistry</i> , 2007, 72, 4001-4011. | 1.7 | 65 |
| 3007 | Rational Design of Minimal Artificial Diels-Alderases Based on the Copper(II) Cation-Aromatic π -Attractive Interaction. <i>Accounts of Chemical Research</i> , 2007, 40, 1049-1055. | 7.6 | 82 |
| 3008 | Aryl to Aryl Palladium Migration in the Heck and Suzuki Coupling of <i>o</i> -Halobiaryls. <i>Journal of the American Chemical Society</i> , 2007, 129, 6298-6307. | 6.6 | 107 |
| 3009 | Density Functional Theory Investigation on the Mechanism of the Hepatitis Delta Virus Ribozyme. <i>Journal of Physical Chemistry B</i> , 2007, 111, 439-445. | 1.2 | 23 |
| 3010 | Electronic and Vibrational Spectroscopies Applied to Organic/Inorganic Interfaces. <i>Chemical Reviews</i> , 2007, 107, 1161-1232. | 23.0 | 149 |
| 3011 | The Conversion among Various B ₄ C Clusters: A Density Functional Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 704-709. | 1.1 | 24 |
| 3012 | Selective Cyclopalladation of R ₃ PNCH ₂ Aryl Iminophosphoranes. <i>Experimental and Computational Study. Inorganic Chemistry</i> , 2007, 46, 10133-10142. | 1.9 | 41 |
| 3013 | New Digermylalkenes and Digermylalkynes: [1,3]-Chlorine Shifts in Organogermanium Chemistry?. <i>Organometallics</i> , 2007, 26, 5136-5139. | 1.1 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3014 | Interstellar Molecule CCCN May Be Formed by Charge-Stripping of [CCCN] ⁺ in the Gas Phase, and When Energized, Undergoes Loss of C with Partial Carbon Scrambling. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12932-12937. | 1.1 | 9 |
| 3015 | Unraveling the Role of Stereo-electronic, Dynamical, and Environmental Effects in Tuning the Structure and Magnetic Properties of Glycine Radical in Aqueous Solution at Different pH Values. <i>Journal of the American Chemical Society</i> , 2007, 129, 15380-15390. | 6.6 | 40 |
| 3016 | Electron-Transfer Induced Repair of 6-4 Photoproducts in DNA: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2351-2361. | 1.1 | 39 |
| 3017 | Theoretical Investigations of Isolated Mo(VI) and Mo(IV) Centers of a Molybdena-Silica Catalyst for Olefin Metathesis. <i>Journal of Physical Chemistry C</i> , 2007, 111, 9337-9348. | 1.5 | 37 |
| 3018 | Self-Sorting Chiral Subcomponent Rearrangement During Crystallization. <i>Journal of the American Chemical Society</i> , 2007, 129, 8774-8780. | 6.6 | 114 |
| 3019 | Cyclization Cascade of Allenyl Azides: A Dual Mechanism. <i>Journal of the American Chemical Society</i> , 2007, 129, 7638-7646. | 6.6 | 35 |
| 3020 | Aggregation of Alkylolithiums in Tetrahydrofuran. <i>Journal of Organic Chemistry</i> , 2007, 72, 2962-2966. | 1.7 | 71 |
| 3021 | How the Central Torsion Angle Affects the Rates of Nonradiative Decay in Some Geometrically Restricted p-Quaterphenyls. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2641-2649. | 1.1 | 18 |
| 3022 | Reversible Redox-Based Optical Sensing of Parts per Million Levels of Nitrosyl Cation in Organic Solvents by Osmium Chromophore-Based Monolayers. <i>Journal of Physical Chemistry C</i> , 2007, 111, 4655-4660. | 1.5 | 21 |
| 3023 | SSOH and HSSO Radicals: An Experimental and Theoretical Study of [S2OH]0/+/- Species. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6526-6533. | 1.1 | 27 |
| 3024 | Helically Annelated and Cross-Conjugated \hat{I}^2 -Oligothiophenes: A Fourier Transform Raman Spectroscopic and Quantum Chemical Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 4854-4860. | 1.5 | 14 |
| 3025 | DFT Studies of Alkene Insertions into Cu ^I -B Bonds in Copper(I) Boryl Complexes. <i>Organometallics</i> , 2007, 26, 2824-2832. | 1.1 | 209 |
| 3026 | A New Look at the Ylidic Bond in Phosphorus Ylides and Related Compounds: Energy Decomposition Analysis Combined with a Domain-Averaged Fermi Hole Analysis. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2859-2869. | 1.1 | 27 |
| 3027 | Creating Quaternary Centers with High Exo Stereoselectivity Using Activated \hat{I}^{\pm} -Alkynyl Dienophiles. <i>Journal of the American Chemical Society</i> , 2007, 129, 10078-10079. | 6.6 | 18 |
| 3028 | Acidity and Proton Affinity of Hypoxanthine in the Gas Phase versus in Solution: Intrinsic Reactivity and Biological Implications. <i>Journal of Organic Chemistry</i> , 2007, 72, 6548-6555. | 1.7 | 48 |
| 3029 | Competition between Hydrogen Abstraction and Halogen Displacement in the Reaction of Br with CH3I, CH3Br, and CH3Cl. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6852-6859. | 1.1 | 5 |
| 3030 | Selective Nucleophilic Chemistry in the Synthesis of 5-Carbamoyl-3-sulfanylmethylisoxazole-4-carboxylic Acids. <i>ACS Combinatorial Science</i> , 2007, 9, 139-142. | 3.3 | 8 |
| 3031 | Chemisorption of Hydrogen Atoms on the Sidewalls of Armchair Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2007, 111, 7376-7383. | 1.5 | 79 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3032 | Oxidative Dehalogenation of Perhalogenated Benzenes by Cytochrome P450 Compound I. <i>Biochemistry</i> , 2007, 46, 5924-5940. | 1.2 | 35 |
| 3033 | Combined Quantum Mechanical and Molecular Mechanical Simulations of One- and Two-Electron Reduction Potentials of Flavin Cofactor in Water, Medium-Chain Acyl-CoA Dehydrogenase, and Cholesterol Oxidase. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5729-5742. | 1.1 | 73 |
| 3034 | Characterization of Co ^{III} -C Bonding in Dichlorovinylcobaloxime Complexes. <i>Inorganic Chemistry</i> , 2007, 46, 1645-1654. | 1.9 | 25 |
| 3035 | Quantum Chemical Modeling of the Oxidation of Dihydroanthracene by the Biomimetic Nonheme Iron Catalyst [(TMC)Fe ^{IV} (O)] ²⁺ . <i>Journal of Physical Chemistry C</i> , 2007, 111, 12397-12406. | 1.5 | 56 |
| 3036 | Mechanisms for NH ₃ Decomposition on the Si(111)-7 × 7 Surface: A DFT Cluster Model Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 16974-16981. | 1.5 | 16 |
| 3037 | Mechanism of the MoO ₂ Cl ₂ -Catalyzed Hydrosilylation: A DFT Study. <i>Inorganic Chemistry</i> , 2007, 46, 10850-10859. | 1.9 | 40 |
| 3038 | Ab initio Study of Ultrafast Photochemical Reaction Dynamics of Phenol Blue. <i>Journal of the American Chemical Society</i> , 2007, 129, 6405-6424. | 6.6 | 13 |
| 3039 | Rhodium Silyl Hydrides in Oxidation State +5: Classical or Nonclassical?. <i>Organometallics</i> , 2007, 26, 4160-4169. | 1.1 | 55 |
| 3040 | In situ UV Resonance Raman Micro-spectroscopic Localization of the Antimalarial Quinine in Cinchona Bark. <i>Journal of Physical Chemistry B</i> , 2007, 111, 4171-4177. | 1.2 | 50 |
| 3041 | Searching for Stable, Five-Coordinate Aquated Al(III) Species. Water Exchange Mechanism and Effect of pH. <i>Inorganic Chemistry</i> , 2007, 46, 1112-1122. | 1.9 | 54 |
| 3042 | A Quantum Mechanical Investigation of Possible Mechanisms for the Nucleotidyl Transfer Reaction Catalyzed by DNA Polymerase I ² . <i>Journal of Physical Chemistry B</i> , 2007, 111, 11244-11252. | 1.2 | 40 |
| 3043 | Bonding and structural characteristics of Zn-, Cu-, and Ni-encapsulated Si clusters: Density-functional theory calculations. <i>Physical Review B</i> , 2007, 75, . | 1.1 | 52 |
| 3044 | Activation of C ₂ H ₆ and C ₃ H ₈ by Gas-Phase Mo ⁺ : Thermochemistry of Mo ⁺ -Ligand Complexes. <i>Organometallics</i> , 2007, 26, 5473-5485. | 1.1 | 23 |
| 3045 | How the Shape of the NH ₂ Group Depends on the Substituent Effect and H-Bond Formation in Derivatives of Aniline. <i>Journal of Physical Chemistry A</i> , 2007, 111, 170-175. | 1.1 | 34 |
| 3046 | Photoinduced H ₂ -Hydrogen Elimination and Radical Formation with CpW(CO) ₃ (CH ₂ CH ₃): Ultrafast IR and DFT Studies. <i>Organometallics</i> , 2007, 26, 1424-1432. | 1.1 | 14 |
| 3047 | Resonance Raman Spectroscopy and Quantum-Chemical Calculations of Push-Pull Molecules: 4-Hydroxy-4-nitroazobenzene and Its Anion. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13452-13456. | 1.1 | 8 |
| 3048 | Atom-Efficient Catalytic Coupling of Imidazolium Salts with Ethylene Involving Ni ^{II} -NHC Complexes as Intermediates: A Combined Experimental and DFT Study. <i>Organometallics</i> , 2007, 26, 5352-5363. | 1.1 | 88 |
| 3049 | Stereoelectronic Substituent Effects in Saturated Main Group Molecules: Severe Problems of Current Kohn-Sham Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 42-45. | 2.3 | 78 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3050 | Relative Antioxidant Efficiency of a Large Series of Carotenoids in Terms of One Electron Transfer Reactions. <i>Journal of Physical Chemistry B</i> , 2007, 111, 12898-12908. | 1.2 | 85 |
| 3051 | Density Functional Theory Study of Triphenyl Phosphite: A Molecular Flexibility and Weak Intermolecular Hydrogen Bonding. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6952-6958. | 1.1 | 11 |
| 3052 | The Reaction Mechanism of Paraoxon Hydrolysis by Phosphotriesterase from Combined QM/MM Simulations. <i>Biochemistry</i> , 2007, 46, 13352-13369. | 1.2 | 137 |
| 3053 | Structural and Electronic Properties of Polyacetylene and Polyynes from Hybrid and Coulomb-Attenuated Density Functionals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11930-11935. | 1.1 | 139 |
| 3054 | The Guanine Tautomer Puzzle: A Quantum Chemical Investigation of Ground and Excited States. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1545-1553. | 1.1 | 169 |
| 3055 | Fast O ₂ Binding at Dicopper Complexes Containing Schiff-Base Dinucleating Ligands. <i>Inorganic Chemistry</i> , 2007, 46, 4997-5012. | 1.9 | 43 |
| 3056 | Assessment of Approximate Density Functional Methods for the Study of the Interactions of Al(III) with Aromatic Amino Acids. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1830-1836. | 2.3 | 8 |
| 3057 | Properties and Spectroscopies. , 0, , 125-312. | | 3 |
| 3058 | High-symmetry high-stability silicon fullerenes: A first-principles study. <i>Physical Review B</i> , 2007, 76, . | 1.1 | 53 |
| 3059 | Theoretical Reinvestigation of the O(3P) + C ₆ H ₆ Reaction: A Quantum Chemical and Statistical Rate Calculations. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3836-3849. | 1.1 | 34 |
| 3060 | Theoretical Survey of the Gas-Phase Reactions of Allylamine with Co ⁺ . <i>Journal of Physical Chemistry A</i> , 2007, 111, 6208-6216. | 1.1 | 15 |
| 3061 | How to Compute Isomerization Energies of Organic Molecules with Quantum Chemical Methods. <i>Journal of Organic Chemistry</i> , 2007, 72, 2118-2126. | 1.7 | 234 |
| 3062 | Electronic Structure of Trigonal-Planar Transition-Metal~Imido Complexes: Spin-State Energetics, Spin-Density Profiles, and the Remarkable Performance of the OLYP Functional. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 689-702. | 2.3 | 110 |
| 3063 | O~O Bond Cleavage in Dinuclear Peroxo Complexes of Iron Porphyrins: A Quantum Chemical Study. <i>Inorganic Chemistry</i> , 2007, 46, 7992-7997. | 1.9 | 13 |
| 3064 | Polarizable Empirical Force Field for the Primary and Secondary Alcohol Series Based on the Classical Drude Model. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1927-1946. | 2.3 | 136 |
| 3065 | Determination of the Absolute Configuration of a Chiral Oxadiazol-3-one Calcium Channel Blocker, Resolved Using Chiral Chromatography, via Concerted Density Functional Theory Calculations of Its Vibrational Circular Dichroism, Electronic Circular Dichroism, and Optical Rotation. <i>Journal of Organic Chemistry</i> , 2007, 72, 4707-4715. | 1.7 | 113 |
| 3066 | Local hybrid functionals: An assessment for thermochemical kinetics. <i>Journal of Chemical Physics</i> , 2007, 127, 194102. | 1.2 | 87 |
| 3067 | An Evaluation of Harmonic Vibrational Frequency Scale Factors. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11683-11700. | 1.1 | 2,264 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3068 | A Density Functional Study of Methanol Clusters. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 54-61. | 2.3 | 128 |
| 3069 | Planarity and Constraint of the Carbonyl Groups in 1,2-Diones Are Determinants for Selective Inhibition of Human Carboxylesterase 1. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 5727-5734. | 2.9 | 37 |
| 3070 | Density Functionals for Noncovalent Interaction Energies of Biological Importance. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 289-300. | 2.3 | 557 |
| 3071 | Double-hybrid density functionals with long-range dispersion corrections: higher accuracy and extended applicability. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 3397. | 1.3 | 979 |
| 3072 | DFT and TD-DFT Calculations on the Electronic Structures and Spectroscopic Properties of Cyclometalated Platinum(II) Complexes. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5465-5472. | 1.1 | 36 |
| 3073 | Fingerprint Vibrational Spectra of Protonated Methyl Esters of Amino Acids in the Gas Phase. <i>Journal of the American Chemical Society</i> , 2007, 129, 2829-2840. | 6.6 | 81 |
| 3074 | Harmonic and Anharmonic Features of IR and NIR Absorption and VCD Spectra of Chiral 4-X-[2.2]Paracyclophanes. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7031-7040. | 1.1 | 26 |
| 3075 | Hydrolysis of <i>N</i> -Sulfinylamines and Isocyanates: A Computational Comparison. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10824-10833. | 1.1 | 18 |
| 3076 | Computational Requirements for Simulating the Structures and Proton Activity of Siliceous Materials. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 593-604. | 2.3 | 17 |
| 3077 | Selective Bromination of Perylene Diimides under Mild Conditions. <i>Journal of Organic Chemistry</i> , 2007, 72, 5973-5979. | 1.7 | 211 |
| 3078 | Kinetic electron emission from Al surfaces by slow ions. <i>Physical Review B</i> , 2007, 75, . | 1.1 | 23 |
| 3079 | Analogy of silicon clusters with deltahedral boranes: How far can it go? Reexamining the structure of Sin and $Sin2^+$, $n=5-13$ clusters. <i>Journal of Chemical Physics</i> , 2007, 127, 244308. | 1.2 | 39 |
| 3080 | Prediction of Gold Zigzag Nanotube-like Structure Based on Au ₃₂ Units: A Quantum Chemical Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 10342-10346. | 1.5 | 39 |
| 3081 | Assessment of Density Functional Theory Methods for the Computation of Heats of Formation and Ionization Potentials of Systems Containing Third Row Transition Metals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6044-6053. | 1.1 | 94 |
| 3082 | Mechanism of S_N2 Disulfide Bond Cleavage by Phosphorus Nucleophiles. Implications for Biochemical Disulfide Reducing Agents. <i>Journal of Organic Chemistry</i> , 2007, 72, 8298-8307. | 1.7 | 84 |
| 3083 | Possible Biotransformation Reactions of Polynuclear Pt(II) Complexes. <i>Inorganic Chemistry</i> , 2007, 46, 2094-2104. | 1.9 | 50 |
| 3084 | Anthracene as a sensitizer for near-infrared luminescence in complexes of Nd(III), Er(III) and Yb(III): an unexpected sensitization mechanism based on electron transfer. <i>Dalton Transactions</i> , 2007, , 1484. | 1.6 | 64 |
| 3085 | Determination of the Absolute Configurations of Natural Products via Density Functional Theory Calculations of Vibrational Circular Dichroism, Electronic Circular Dichroism, and Optical Rotation: The Iridoids Plumericin and Isoplumericin. <i>Journal of Organic Chemistry</i> , 2007, 72, 3521-3536. | 1.7 | 97 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3086 | Determination of the Absolute Configurations of Natural Products via Density Functional Theory Calculations of Vibrational Circular Dichroism, Electronic Circular Dichroism and Optical Rotation: The Schizogyane Alkaloid Schizogyne. <i>Journal of Organic Chemistry</i> , 2007, 72, 2508-2524. | 1.7 | 100 |
| 3087 | Experimental and Computational Studies of Nuclear Substituted 1,1-Dimethyl-2,2-Bipyridinium Tetrafluoroborates. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13567-13574. | 1.1 | 29 |
| 3088 | Theoretical Methods for Computing Enthalpies of Formation of Gaseous Compounds. <i>Reviews in Computational Chemistry</i> , 2007, , 147-211. | 1.5 | 31 |
| 3089 | DFT Calculations on the Spin-Crossover Complex Fe(salen)(NO): A Quest for the Best Functional. <i>Journal of Physical Chemistry B</i> , 2007, 111, 12621-12624. | 1.2 | 183 |
| 3090 | Computational Electrochemistry: The Aqueous Ru ³⁺ Ru ²⁺ -Reduction Potential. <i>Journal of Physical Chemistry C</i> , 2007, 111, 5783-5799. | 1.5 | 126 |
| 3091 | Theory and computation of nuclear magnetic resonance parameters. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5399. | 1.3 | 226 |
| 3092 | Design of Tetrathiafulvalene-Based Phosphazenes Combining a Good Electron-Donor Capacity and Possible Inclusion Adduct Formation (Part II). <i>Journal of Physical Chemistry C</i> , 2007, 111, 4838-4846. | 1.5 | 29 |
| 3093 | Critical Role of the Correlation Functional in DFT Descriptions of an Agostic Niobium Complex. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1329-1336. | 2.3 | 52 |
| 3094 | Electronic differentiation competes with transition state sensitivity in palladium-catalyzed allylic substitutions. <i>Beilstein Journal of Organic Chemistry</i> , 2007, 3, 36. | 1.3 | 5 |
| 3095 | The Water-Exchange Mechanism of the [UO ₂ (OH) ₂] ²⁺ Ion Revisited: The Importance of a Proper Treatment of Electron Correlation. <i>Chemistry - A European Journal</i> , 2007, 13, 800-811. | 1.7 | 44 |
| 3096 | Reaction Chemistry of Complexes Containing Pt η^2 H, Pt η^2 SH, or Pt η^2 S Fragments: From Their Apparent Simplicity to the Maze of Reactions Underlying Their Interconversion. <i>Chemistry - A European Journal</i> , 2007, 13, 1047-1063. | 1.7 | 17 |
| 3097 | A Valuable, Inexpensive CuI/N-Heterocyclic Carbene Catalyst for the Selective Diboration of Styrene. <i>Chemistry - A European Journal</i> , 2007, 13, 2614-2621. | 1.7 | 156 |
| 3098 | 2,2-Biphosphinines and 2,2-Bipyridines in Homoleptic Dianionic Group η^4 Complexes and Neutral 2,2-Biphosphinine Group η^6 d ₆ Metal Complexes: Octahedral versus Trigonal-Prismatic Geometries. <i>Chemistry - A European Journal</i> , 2007, 13, 2953-2965. | 1.7 | 13 |
| 3099 | Synthesis and Characterization of Monodisperse Oligo(flourene-co-bithiophene)s. <i>Chemistry - A European Journal</i> , 2007, 13, 6238-6248. | 1.7 | 38 |
| 3100 | New Modes of Reactivity in the Threshold of the Reduction Potential in Solution. Alkylation of Lithium PAH (Polycyclic Aromatic Hydrocarbon) Dianions by Primary Fluoroalkanes: A Reaction Pathway Complementing the Classical Birch Reductive Alkylation. <i>Chemistry - A European Journal</i> , 2007, 13, 10096-10107. | 1.7 | 28 |
| 3101 | Can [M(H) ₂ (H ₂)(PXP)] Pincer Complexes (M=Fe, Ru, Os; X=N, O, S) Serve as Catalyst Lead Structures for NH ₃ Synthesis from N ₂ and H ₂ ? <i>Chemistry - A European Journal</i> , 2007, 13, 6636-6643. | 1.7 | 37 |
| 3102 | Evidence for Spontaneous Release of Acrylates from a Transition-Metal Complex Upon Coupling Ethene or Propene with a Carboxylic Moiety or CO ₂ . <i>Chemistry - A European Journal</i> , 2007, 13, 9028-9034. | 1.7 | 61 |
| 3103 | How Strong Are Hydrogen Bonds in Metalla η^2 -diketones?. <i>Chemistry - A European Journal</i> , 2007, 13, 9668-9678. | 1.7 | 25 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3104 | Estimation of the Kinetic Acidity from Substrate Conformation – Stereochemical Course of the Deprotonation of Cyclohexenyl Carbamates. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 1645-1649. | 7.2 | 18 |
| 3105 | Revisiting the Electronic Ground State of Copper Corroles. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 445-448. | 7.2 | 154 |
| 3106 | Synthesis and Characterization of (Z)-[N3NFO] ⁺ and (E)-[N3NFO] ⁺ . <i>Angewandte Chemie - International Edition</i> , 2007, 46, 3023-3027. | 7.2 | 12 |
| 3107 | The Generation of Aryl Anions by Double Electron Transfer to Aryl Iodides from a Neutral Ground-State Organic Super-Electron Donor. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 5178-5183. | 7.2 | 123 |
| 3108 | Sixty Years after Wittig: Gas-Phase Synthesis of Lithium Trimethylammonium Methylide, [(CH ₃) ₃ NCH ₂ Li] ⁺ . <i>Angewandte Chemie - International Edition</i> , 2007, 46, 7048-7051. | 7.2 | 27 |
| 3109 | Formation and Structure of the [(1,2- ⁶ H ₄ PC ₂ Sb) ₂] ⁴⁺ Ion: Implications for an Extended Family of Isoelectronic Main-Group Radicals. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 7827-7830. | 7.2 | 26 |
| 3110 | Boryl-substituted 1-silacyclobutenes. Formation and molecular structure. <i>Applied Organometallic Chemistry</i> , 2007, 21, 39-45. | 1.7 | 20 |
| 3115 | Sixty Years after Wittig: Gas-Phase Synthesis of Lithium Trimethylammonium Methylide, [(CH ₃) ₃ NCH ₂ Li] ⁺ . <i>Angewandte Chemie</i> , 2007, 119, 7178-7181. | 1.6 | 12 |
| 3117 | The Stereostructure of Porphyrin-334: An Experimental and Computational NMR Investigation. Evidence for an Efficient ¹ H Proton Sponge™. <i>Helvetica Chimica Acta</i> , 2007, 90, 488-511. | 1.0 | 47 |
| 3118 | Donor/Acceptor Effects on the Linear and Nonlinear Optical Properties of Geminal Diethynylethenes (g-DEEs). <i>Helvetica Chimica Acta</i> , 2007, 90, 909-927. | 1.0 | 23 |
| 3119 | Aromaticity in linear polyacenes: Generalized population analysis and molecular quantum similarity approach. <i>Journal of Computational Chemistry</i> , 2007, 28, 152-160. | 1.5 | 51 |
| 3120 | Theoretical study of the electronic spectra of oxidized and reduced states of lumiflavin and its derivative. <i>Journal of Computational Chemistry</i> , 2007, 28, 727-739. | 1.5 | 36 |
| 3121 | A systematic quantum chemical investigation of the C-H bond activation in methane by gas phase vanadium oxide cation VO ⁺ . <i>Journal of Computational Chemistry</i> , 2007, 28, 2252-2259. | 1.5 | 10 |
| 3122 | Electric field effects on the performance of a candidate multipole molecular switch: A quantum computational study. <i>Journal of Computational Chemistry</i> , 2007, 28, 922-931. | 1.5 | 23 |
| 3123 | Energy landscapes of nucleophilic substitution reactions: A comparison of density functional theory and coupled cluster methods. <i>Journal of Computational Chemistry</i> , 2007, 28, 1551-1560. | 1.5 | 89 |
| 3124 | Implementation of divide-and-conquer method including Hartree-Fock exchange interaction. <i>Journal of Computational Chemistry</i> , 2007, 28, 2003-2012. | 1.5 | 130 |
| 3125 | Description of core excitations by time-dependent density functional theory with local density approximation, generalized gradient approximation, meta-generalized gradient approximation, and hybrid functionals. <i>Journal of Computational Chemistry</i> , 2007, 28, 2067-2074. | 1.5 | 43 |
| 3126 | Electron affinities of heavier phosphoryl and thiophosphoryl halides APX ₃ (A = O, S and X = Br, I). <i>Journal of Computational Chemistry</i> , 2007, 28, 2027-2033. | 1.5 | 2 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3127 | Model transition states for methane diazonium ion methylation of guanine runs in oligomeric DNA. <i>Journal of Computational Chemistry</i> , 2007, 28, 2352-2365. | 1.5 | 11 |
| 3128 | Host-Guest Complexes of Oligopyridine Cryptands: Prediction of Ion Selectivity by Quantum Chemical Calculations. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 1120-1127. | 1.0 | 26 |
| 3129 | CO ₂ Fixation by Alkylzinc Amides: A Quantum Chemical Study Motivated by Recent Experimental Results. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 675-683. | 1.0 | 13 |
| 3130 | Synthesis, Structure and Reactivity of Trimethylsilyl-Substituted Phosphametalloenes. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 553-561. | 1.0 | 17 |
| 3131 | Ligand-Exchange Processes on Solvated Lithium Cations: Acetonitrile and Hydrogen Cyanide. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 1815-1822. | 1.0 | 36 |
| 3132 | Syntheses, Characterization and Reactivity of Iron(II), Nickel(II), Copper(II) and Zinc(II) Complexes of the Ligand N,N,N',N'-Tetrakis(2-pyridylmethyl)benzene-1,3-diamine (1,3-tpbd) and Its Phenol Derivative 2,6-Bis[bis(2-pyridylmethyl)amino]-p-cresol (2,6-tpcd). <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 429-443. | 1.0 | 20 |
| 3133 | Systematic Counterion Tuning of the Solid-State Structure of [Pt(thiourea) ₄] ²⁺ . <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 1390-1404. | 1.0 | 11 |
| 3134 | Ligand Exchange Processes on Solvated Lithium Cations: Complexation by Cryptands in Acetone as Solvent. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 3067-3076. | 1.0 | 10 |
| 3135 | The Role of Water in the Stereoselective Hydrogenation of 1,2-Diphenylacetylene Catalyzed by the Water-Soluble [RuCl ₂ (mtpmms) ₂] ₂ . <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 2879-2889. | 1.0 | 14 |
| 3136 | A Linear Ru-Tl-Ru Complex Obtained from Halide Abstraction: An Example of Metal-Dative Bonding. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 3240-3246. | 1.0 | 16 |
| 3137 | Purines Bearing Phenanthroline or Bipyridine Ligands and Their Ru(II) Complexes in Position 8 as Model Compounds for Electrochemical DNA Labeling – Synthesis, Crystal Structure, Electrochemistry, Quantum Chemical Calculations, Cytostatic and Antiviral Activity. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 1752-1769. | 1.0 | 45 |
| 3138 | Mixed Titanium-Hafnium Chloridometallate Complexes. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 2434-2442. | 1.0 | 7 |
| 3139 | C-S Bond Activation and Partial Hydrogenation of Thiophene by a Dinuclear Trihydride Platinum Complex. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 5707-5719. | 1.0 | 17 |
| 3140 | Planar Chiral (Arene)chromiumcarbonyl-Substituted Propargyl Cations – A Spectroscopic and Computational Study. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 540-547. | 1.2 | 6 |
| 3141 | Base-Catalyzed Anti-Markovnikov Hydroamination of Vinylarenes – Scope, Limitations and Computational Studies. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 3311-3325. | 1.2 | 84 |
| 3142 | Why are Phosphole Oxides Unstable? The Phenomenon of Antiaromaticity as a Destabilizing Factor. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 4765-4771. | 1.2 | 23 |
| 3143 | Photochemical Generation and Reactivity of Naphthyl Cations: <i>cine</i> Substitution. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 5353-5363. | 1.2 | 17 |
| 3144 | Stereospecific Side Chain Activation in Cyclobutadiene-Fe(CO) ₃ Chemistry: A Theoretical and Experimental Study on the Structure and Configurational Stability of Cationic, Radical and Anionic Intermediates. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 3991-3998. | 1.2 | 7 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3145 | New [4.4]Cyclophane Diketals, Monoketones, and Diketones: Design, Synthesis, and Structural Analysis. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 4674-4687. | 1.2 | 6 |
| 3146 | Carbolithiation of Simple Terminal and Strained Internal Alkenes by the Naphthalene and the Biphenyl Dianion: New Modes of Reactivity of Highly Reduced Organic Species in Solution. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 5514-5526. | 1.2 | 24 |
| 3147 | Insights into the Molecular Structure and Reactivity of β -Dialkoxy-Substituted Ethyne and Butadiyne. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 5834-5839. | 1.2 | 10 |
| 3148 | Theoretical Study on the Reaction Mechanism of Ketene CH_2CO with Isocyanate NCO Radical. <i>Chinese Journal of Chemistry</i> , 2007, 25, 1105-1111. | 2.6 | 2 |
| 3149 | Kinetic Study on the Reaction of OH Radical with Dimethyl Sulfide in the Absence of Oxygen. <i>ChemPhysChem</i> , 2007, 8, 255-263. | 1.0 | 11 |
| 3150 | On the Origin of Red and Blue Shifts of C-H and C=C Stretching Vibrations in Formic Acid (Formate) Tj ETQq1 1 0,784314.rgBT /Ove | 1.0 | 28 |
| 3151 | Exploration of the Ca^{2+} Interaction Modes of the Nifedipine Calcium Channel Antagonist. <i>ChemPhysChem</i> , 2007, 8, 304-314. | 1.0 | 4 |
| 3152 | Ligand-Exchange Processes on Solvated Lithium Cations: DMSO and Water/DMSO Mixtures. <i>ChemPhysChem</i> , 2007, 8, 1315-1320. | 1.0 | 41 |
| 3153 | Luminescent Eu(III) and Gd(III) Trisbipyridine Cryptates: Experimental and Theoretical Study of the Substituent Effects. <i>ChemPhysChem</i> , 2007, 8, 480-488. | 1.0 | 48 |
| 3154 | Fourier Transform Raman and DFT Study of Three Annulated Oligothiophenes with Different Molecular Shapes. <i>ChemPhysChem</i> , 2007, 8, 745-750. | 1.0 | 6 |
| 3155 | Theoretical Prediction and the First IR Matrix Observation of Several-L-Cysteine Molecule Conformers. <i>ChemPhysChem</i> , 2007, 8, 1085-1094. | 1.0 | 61 |
| 3156 | Icosahedral and Ring-Shaped Allotropes of Arsenic. <i>ChemPhysChem</i> , 2007, 8, 2373-2378. | 1.0 | 17 |
| 3157 | A DFT Study of the Nitric Oxide and Tyrosyl Radical Interaction: A Proposed Radical Mechanism. <i>ChemPhysChem</i> , 2007, 8, 2595-2602. | 1.0 | 6 |
| 3158 | 1-Cyclohepta-2,4,6-trienyl-selanes ^{77}Se NMR study: Indirect nuclear ^{77}Se ^{13}C spin-spin coupling constants and application of density functional theory (DFT) calculations. <i>Magnetic Resonance in Chemistry</i> , 2007, 45, 198-204. | 1.1 | 25 |
| 3159 | Comparison of various density functional methods for distinguishing stereoisomers based on computed ^1H or ^{13}C NMR chemical shifts using diastereomeric penam β -lactams as a test set. <i>Magnetic Resonance in Chemistry</i> , 2007, 45, 819-829. | 1.1 | 46 |
| 3160 | Adsorption and thermal chemistry of 1,1,1,5,5,5-hexafluoro-2,4-pentanedione (hfacH) and (hexafluoroacetylacetonate)Cu(vinyltrimethylsilane) ((hfac)Cu(VTMS)) on TiCN-covered Si(100) surface. <i>Surface Science</i> , 2007, 601, 155-164. | 0.8 | 22 |
| 3161 | The molecular orientation of DNA bases on H-passivated Si(111) surfaces investigated by means of near edge X-ray absorption fine structure spectroscopy. <i>Surface Science</i> , 2007, 601, 2291-2296. | 0.8 | 16 |
| 3162 | Properties and metathesis activity of monomeric and dimeric Mo centres variously located on γ -alumina β -Al ₂ O ₃ . A DFT study. <i>Surface Science</i> , 2007, 601, 2054-2065. | 0.8 | 35 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3163 | Structure modification of maltol (3-hydroxy-2-methyl-4H-pyran-4-one) upon cation and anion formation studied by vibrational spectroscopy and quantum-mechanical calculations. <i>Vibrational Spectroscopy</i> , 2007, 43, 344-350. | 1.2 | 10 |
| 3164 | Mixed aggregates of dilithiodiamines with alkyllithiums and lithium enolates. <i>Tetrahedron</i> , 2007, 63, 1331-1338. | 1.0 | 8 |
| 3165 | Kinetic resolution of racemic alcohols catalyzed by minimal artificial acylases derived from l-histidine. <i>Tetrahedron</i> , 2007, 63, 6191-6203. | 1.0 | 49 |
| 3166 | Lithium 2,3-dihydro-1-benzothiophene-1,1-dioxide: synthesis, characterization, DFT calculations, and reactivity toward aldehydes and azomethines. <i>Tetrahedron</i> , 2007, 63, 11122-11134. | 1.0 | 5 |
| 3167 | Phosphine triggered [3+2] allenoate acrylate annulation: a mechanistic enlightenment. <i>Tetrahedron Letters</i> , 2007, 48, 3617-3620. | 0.7 | 172 |
| 3168 | Metal complexation of protocatechuic acid and its derivatives: Determination of the optimal computational conditions for the simulation of electronic spectra. <i>Computational and Theoretical Chemistry</i> , 2007, 806, 131-140. | 1.5 | 12 |
| 3169 | A density functional theory study of the mechanism of the Paal-Knorr pyrrole synthesis. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 97-107. | 1.5 | 30 |
| 3170 | Theoretical study on the reaction of W ⁺ with CO ₂ in the gas phase. <i>Computational and Theoretical Chemistry</i> , 2007, 807, 49-54. | 1.5 | 4 |
| 3171 | Modeling lithium dialkylamides in ethereal solvents: A test of the microsolvation model. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 191-196. | 1.5 | 25 |
| 3172 | Theoretical studies on the geometry, vibrational frequencies and electronic properties of [X(OH) ₆ Mo ₆ O ₁₈] ⁴⁻ /3 ⁻ (X=FeII/CoIII) Anderson-type anions. <i>Computational and Theoretical Chemistry</i> , 2007, 809, 1-10. | 1.5 | 9 |
| 3173 | Cysteine conformations revisited. <i>Computational and Theoretical Chemistry</i> , 2007, 810, 129-134. | 1.5 | 65 |
| 3174 | A computational investigation of the retrocyclization reaction of silacyclo-but-2-enes to 1-silabuta-1,3-dienes: Focus on the effect of the substituents. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 153-160. | 1.5 | 8 |
| 3175 | A theoretical study on tautomerization processes of dehydrated and monohydrated cytosine. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 161-167. | 1.5 | 29 |
| 3176 | The H ₂ -hydrogenation of ketones catalysed by ruthenium(II) complexes: A density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2007, 812, 39-49. | 1.5 | 33 |
| 3177 | Reaction of NH(3 ⁺) radical with C ₂ H ₄ : A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2007, 816, 21-29. | 1.5 | 2 |
| 3178 | Preferred conformations of the gas phase complex between Li ⁺ and a model macrocycle tetraamide. <i>Computational and Theoretical Chemistry</i> , 2007, 819, 79-87. | 1.5 | 4 |
| 3179 | Ionization of carbonyl sulphide/disulphur monoxide mixtures in atmospheric gases: A theoretical study of the formation of S ₃ O ⁺ ions. <i>Computational and Theoretical Chemistry</i> , 2007, 822, 153-157. | 1.5 | 0 |
| 3180 | Theoretical investigation of the potential energy surface for the N(4S)+C ₂ H ₃ reaction via density functional theory and ab initio molecular electronic structure theory. <i>Computational and Theoretical Chemistry</i> , 2007, 847, 79-85. | 1.5 | 1 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3181 | An investigation of the surface-enhanced Raman scattering (SERS) effect from laser irradiation of Ag nanoparticles prepared by trisodium citrate reduction method. <i>Applied Surface Science</i> , 2007, 253, 4450-4455. | 3.1 | 19 |
| 3182 | Theoretical study of 5-aminolevulinic acid (5ALA) and some pharmaceutically important derivatives. <i>Chemical Physics Letters</i> , 2007, 434, 101-106. | 1.2 | 4 |
| 3183 | Clusters of glycolic acid and 16 water molecules. <i>Chemical Physics Letters</i> , 2007, 434, 176-181. | 1.2 | 19 |
| 3184 | A computational study of the molecular structure of 1,3,4,2,4-benzodithiadiazine. <i>Chemical Physics Letters</i> , 2007, 434, 200-204. | 1.2 | 6 |
| 3185 | A reparametrization of a meta-GGA exchange-correlation functional with improved descriptions of van der Waals interactions. <i>Chemical Physics Letters</i> , 2007, 436, 394-399. | 1.2 | 6 |
| 3186 | The functionalization of (5, 5), (9, 0), and (10, 0) single wall carbon nanotubes by CH _n fragments. <i>Chemical Physics Letters</i> , 2007, 437, 99-103. | 1.2 | 10 |
| 3187 | Treatment of singlet-triplet splitting of a set of phenylene ethylenes organic molecules by TD-DFT. <i>Chemical Physics Letters</i> , 2007, 439, 236-242. | 1.2 | 13 |
| 3188 | The performances of a parameter-free local correlation functional: The Ragot-Cortona model. <i>Chemical Physics Letters</i> , 2007, 439, 381-385. | 1.2 | 19 |
| 3189 | Local hybrid exchange-correlation functionals based on the dimensionless density gradient. <i>Chemical Physics Letters</i> , 2007, 440, 160-168. | 1.2 | 98 |
| 3190 | Assignment of the lowest-lying THz absorption signatures in biotin and lactose monohydrate by solid-state density functional theory. <i>Chemical Physics Letters</i> , 2007, 440, 203-209. | 1.2 | 101 |
| 3191 | A B3LYP study on the mechanism of second H ₂ O formation in a fully reduced cytochrome c oxidase. <i>Chemical Physics Letters</i> , 2007, 440, 296-301. | 1.2 | 7 |
| 3192 | $\dot{\text{I}}^2$ -Scission of thioimidoyl radicals (R1-N-CS-R2): A theoretical scale of radical leaving group ability. <i>Chemical Physics Letters</i> , 2007, 443, 383-388. | 1.2 | 9 |
| 3193 | On the insertion mechanism of molecular oxygen into a Pd(II)-H bond. Something to add. <i>Chemical Physics Letters</i> , 2007, 443, 183-189. | 1.2 | 25 |
| 3194 | Adsorption structures of thiophene on Si(100)-(2 \times 1) studied by scanning tunneling microscopy and density functional theory. <i>Chemical Physics Letters</i> , 2007, 443, 347-351. | 1.2 | 15 |
| 3195 | Theoretical investigation for the reaction of NO ₂ with CO catalyzed by Sc ⁺ . <i>Chemical Physics Letters</i> , 2007, 446, 8-13. | 1.2 | 17 |
| 3196 | Comparative study of copper(II)-curcumin complexes as superoxide dismutase mimics and free radical scavengers. <i>European Journal of Medicinal Chemistry</i> , 2007, 42, 431-439. | 2.6 | 151 |
| 3197 | Electronic transitions and bonding properties in a series of five-coordinate d^6 -electron complexes [Mn(CO) ₃ (L ₂)] ⁺ (L ₂ =chelating redox-active π -donor ligand). <i>Coordination Chemistry Reviews</i> , 2007, 251, 557-576. | 9.5 | 63 |
| 3198 | Interconfigurational energies and ionization potentials: Test of a correlation energy functional. <i>Chemical Physics</i> , 2007, 337, 161-167. | 0.9 | 16 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3199 | Structural and electronic characteristics of perhydrogenated carbon nanotubes. <i>Chemical Physics</i> , 2007, 340, 120-126. | 0.9 | 9 |
| 3200 | Metal-ligand bonding in metallocenes: Differentiation between spin state, electrostatic and covalent bonding. <i>Inorganica Chimica Acta</i> , 2007, 360, 179-189. | 1.2 | 192 |
| 3201 | Mechanism of the gas phase reactions of the C ₅ H ₅ Ni ⁺ and C ₅ H ₅ Co ⁺ ions with substituted pyridines. A combined experimental and theoretical study. <i>Inorganica Chimica Acta</i> , 2007, 360, 1170-1182. | 1.2 | 2 |
| 3202 | The platinum complexes with histamine: Pt(II)(Hist)Cl ₂ , Pt(II)(Iodo-Hist)Cl ₂ and Pt(IV)(Hist) ₂ Cl ₂ . <i>Inorganica Chimica Acta</i> , 2007, 360, 1902-1914. | 1.2 | 26 |
| 3203 | Proton and hydrogen atom adducts to cytosine. An experimental and computational study. <i>International Journal of Mass Spectrometry</i> , 2007, 265, 106-123. | 0.7 | 33 |
| 3204 | Vacuum electrospray ionization study of the ionic liquid, [Emim][Im]. <i>International Journal of Mass Spectrometry</i> , 2007, 265, 146-158. | 0.7 | 67 |
| 3205 | Cytosine neutral molecules and cation radicals in the gas-phase. <i>International Journal of Mass Spectrometry</i> , 2007, 267, 30-42. | 0.7 | 61 |
| 3206 | Quantum chemical calculations on the structure and stability of Mg ²⁺ +XH ₃ OH complexes in the gas phase (X=C, Si, and Ge). <i>International Journal of Mass Spectrometry</i> , 2007, 263, 267-275. | 0.7 | 10 |
| 3207 | Charged titanium-doped carbon clusters: Structures and energetics. <i>International Journal of Mass Spectrometry</i> , 2007, 266, 50-61. | 0.7 | 25 |
| 3208 | Hydrogen bonds and electrostatic interactions in 1:1 and 2:1 complexes of homarine with mineral acids studied by NMR, FTIR, DFT and X-ray diffraction. <i>Journal of Molecular Structure</i> , 2007, 827, 56-66. | 1.8 | 13 |
| 3209 | Crystal and molecular structure of 4-carboxypiperidinium chloride (4-piperidinecarboxylic acid) Tj ETQqO 0 0 rgBT /Overlock 10 Tf 50 342 | 1.8 | 419 |
| 3210 | Spectroscopic properties of N-n-butyltetrachlorophthalimide and supramolecular interactions in its crystals. <i>Journal of Molecular Structure</i> , 2007, 833, 197-202. | 1.8 | 13 |
| 3211 | Vibrational spectra of oligothieryl-vinylenes with donor-acceptor and donor-acceptor substitution patterns. <i>Journal of Molecular Structure</i> , 2007, 834-836, 374-379. | 1.8 | 1 |
| 3212 | Crystal and molecular structure, hydrogen bonding and electrostatic interactions of bis(homarine) hydrogen perchlorate studied by X-ray diffraction, DFT calculations, FTIR and Raman spectroscopies. <i>Journal of Molecular Structure</i> , 2007, 839, 99-106. | 1.8 | 27 |
| 3213 | Vibrational spectra of nonlinear optical chromophores based on octopolar C ₃ -symmetric 1,3,5 trisalkynylbenzenes. <i>Journal of Molecular Structure</i> , 2007, 834-836, 369-373. | 1.8 | 2 |
| 3214 | X-ray, MP2 and DFT studies of the structure, vibrational and NMR spectra of homarine. <i>Journal of Molecular Structure</i> , 2007, 846, 1-12. | 1.8 | 23 |
| 3215 | Formation of N,N,N',N'-tetramethylformamidinium disulphide from the chemical and electrochemical oxidation of tetramethylthiourea: Vibrational spectra and crystal structure of the chloride dihydrate salt. <i>Journal of Molecular Structure</i> , 2007, 871, 131-139. | 1.8 | 5 |
| 3216 | X-ray and ab initio studies of the structure, vibrational and NMR spectra of 1-methyl-3-hydroxypyridinium chloride. <i>Journal of Molecular Structure</i> , 2007, 844-845, 102-114. | 1.8 | 8 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 3217 | Structure of 1-methylpyridinium-4-carboxylate monohydrate studied by X-ray, FT-IR, Raman, NMR and ab initio methods. <i>Journal of Molecular Structure</i> , 2007, 844-845, 140-156. | 1.8 | 17 |
| 3218 | Multinuclear NMR and DFT studies of the structure and fluxionality for M(EDTA) ⁿ⁻ , M=Al, Ga and In in solution. <i>Journal of Molecular Liquids</i> , 2007, 131-132, 72-80. | 2.3 | 6 |
| 3219 | Molecular structure, hydrogen bonding, basicity and spectroscopic properties of 3-hydroxypyridine betaine hydrochloride monohydrate. <i>Journal of Molecular Structure</i> , 2007, 832, 63-72. | 1.8 | 5 |
| 3220 | Theory of complicated liquids Investigation of liquids, solvents and solvent effects with modern theoretical methods. <i>Physics Reports</i> , 2007, 440, 1-111. | 10.3 | 67 |
| 3221 | The effects of steric aliphatic interactions in the coordination polymer of bis(N,N-diethylglycinato)copper(II): Experimental evidence and theoretical modeling. <i>Polyhedron</i> , 2007, 26, 1087-1097. | 1.0 | 4 |
| 3222 | 1-D Polymeric divalent metal m-ferrocenylbenzoates: Structures, NLO and electrochemical properties. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 1584-1592. | 0.8 | 21 |
| 3223 | Mechanism of olefin hydrosilylation catalyzed by [RuCl(NCCH ₃) ₅] ⁺ : A DFT study. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 2282-2290. | 0.8 | 30 |
| 3224 | Dianionic amidinates at silicon and germanium centers: Four-, six- and eight-membered rings. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 2789-2799. | 0.8 | 12 |
| 3225 | Synthesis, characterization and studies on DNA-binding of a new Cu(II) complex with N1,N8-bis(1-methyl-4-nitropyrrole-2-carbonyl)triethylenetetramine. <i>Journal of Inorganic Biochemistry</i> , 2007, 101, 10-18. | 1.5 | 192 |
| 3226 | Theoretical investigations of the hydrolysis pathway of verdoheme to biliverdin. <i>Journal of Inorganic Biochemistry</i> , 2007, 101, 385-395. | 1.5 | 18 |
| 3227 | Theoretical study on electronic structures of FeOO, FeOOH, FeO(H ₂ O), and FeO in hemes: As intermediate models of dioxygen reduction in cytochrome c oxidase. <i>Journal of Inorganic Biochemistry</i> , 2007, 101, 1410-1427. | 1.5 | 24 |
| 3228 | A theoretical study of the principles regulating the specificity for Al(III) against Mg(II) in protein cavities. <i>Journal of Inorganic Biochemistry</i> , 2007, 101, 1192-1200. | 1.5 | 31 |
| 3229 | Kinetics for the reaction of phenyl radical with phenylacetylene and styrene. <i>Proceedings of the Combustion Institute</i> , 2007, 31, 249-256. | 2.4 | 12 |
| 3230 | Oxidation pathways in the reaction of diacetylene with OH radicals. <i>Proceedings of the Combustion Institute</i> , 2007, 31, 185-192. | 2.4 | 20 |
| 3231 | Comparison between optimized geometries and vibrational frequencies calculated by the DFT methods for the Anderson-type heteropolyanion: Hexamolybdoaluminate(III), [Al _{III} (OH) ₆ Mo ₆ O ₁₈] ₃ ^{a-} . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 66, 1126-1132. | 2.0 | 3 |
| 3232 | A DFT conformational analysis and VCD study on methyl tetrahydrofuran-2-carboxylate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 67, 402-411. | 2.0 | 31 |
| 3233 | The study of resonance Raman scattering spectrum on the surface of Cu nanoparticles with ultraviolet excitation and density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 67, 767-771. | 2.0 | 10 |
| 3234 | FT-IR and NMR investigation of 1-phenylpiperazine: A combined experimental and theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 67, 793-801. | 2.0 | 52 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3235 | FT-IR and NMR investigation of 2-(1-cyclohexenyl)ethylamine: A combined experimental and theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 68, 55-62. | 2.0 | 14 |
| 3236 | Electron capture in spin-trap capped peptides. An experimental example of ergodic dissociation in peptide cation-radicals. <i>Journal of the American Society for Mass Spectrometry</i> , 2007, 18, 432-444. | 1.2 | 37 |
| 3237 | N,N,N',N'-Triphenylguanidinium trifluoroacetate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2007, 63, o501-o503. | 0.2 | 7 |
| 3238 | Hydrolysis and Oxidation of a 1-Boryl-1-silyl-alkene. Molecular Structures of 9-Hydroxy-9-borabicyclo[3.3.1]nonane and a Bicyclic Oxasilaboro-heptadecane B ₂ (OSiPh ₂ OSiPh ₂ O) ₃ . <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2007, 633, 453-457. | 0.6 | 5 |
| 3239 | Stanna-closo-dodecaborate: The Crystal Structure of [Li(thf) ₃] ₂ [SnB ₁₁ H ₁₁], Vibrational Spectroscopy, Thermal Analysis and DFT Calculations. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2007, 633, 693-699. | 0.6 | 12 |
| 3240 | Syntheses of N-(Diphenylphosphanyl)-2-pyridylmethylamine and Its Use as a Ligand in Magnesium and Zinc Complexes. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2007, 633, 893-902. | 0.6 | 17 |
| 3241 | On the Mechanism of CO ₂ Insertion into the Mg-N Bond of Molecular Mono- and Dinuclear Magnesium Compounds: A Quantum Chemical Study. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2007, 633, 2191-2198. | 0.6 | 10 |
| 3242 | The New Si^{6-} Silicate Dianion [Si(NCO) ₆] ²⁻ : Synthesis and Structural Characterization of [K(18-crown-6)] ₂ [Si(NCO) ₆]. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2007, 633, 2667-2670. | 0.6 | 17 |
| 3243 | Light-induced cytotoxicity of 16 polycyclic aromatic hydrocarbons on the US EPA priority pollutant list in human skin HaCaT keratinocytes: Relationship between phototoxicity and excited state properties. <i>Environmental Toxicology</i> , 2007, 22, 318-327. | 2.1 | 40 |
| 3244 | Analysis of self-interaction correction for describing core excited states. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 23-29. | 1.0 | 43 |
| 3245 | Comparative semiempirical and ab initio study of the structural and chemical properties of uric acid and its anions. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 172-181. | 1.0 | 15 |
| 3246 | Theoretical study of the reaction of alkynes with furan catalyzed by AuCl ₃ and AuCl. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 359-365. | 1.0 | 29 |
| 3247 | Theoretical study of XCN ⁻ (X = F, Cl) anions. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 680-684. | 1.0 | 2 |
| 3248 | Spectroscopic constants and molecular properties of rare-gas diatomic molecule in Lennard-Jones potential: Ab initio and density functional study. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 824-831. | 1.0 | 7 |
| 3249 | Theoretical study of spectroscopic constants and molecular properties of rare-gas diatomic cations. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1067-1072. | 1.0 | 2 |
| 3250 | DFT study of rearrangements in cyclopentylheptyl carbocations. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1772-1781. | 1.0 | 8 |
| 3251 | Six-coordinate Co ²⁺ with imidazole, NH ₃ , and H ₂ O ligands: Approaching spin crossover. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1415-1429. | 1.0 | 2 |
| 3252 | Effect of tube length on the chemisorptions of one and two hydrogen atoms on the sidewalls of (3,3) and (4,4) single-walled carbon nanotubes: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 2211-2219. | 1.0 | 32 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 3253 | Ab initio and DFT study of La ³⁺ hydration. International Journal of Quantum Chemistry, 2007, 107, 2353-2360. | 1.0 | 13 |
| 3254 | Quantum chemical study of penicillin: Reactions after acylation. International Journal of Quantum Chemistry, 2007, 107, 2032-2039. | 1.0 | 2 |
| 3255 | Application of the ONIOM (QM/QM) method in the study of molybdena-silica system active in olefin metathesis. International Journal of Quantum Chemistry, 2007, 107, 2111-2119. | 1.0 | 20 |
| 3256 | Investigation of strain relaxation mechanism in small SiGe clusters. Physica Status Solidi (B): Basic Research, 2007, 244, 3601-3611. | 0.7 | 6 |
| 3257 | Theoretical studies of ethylene addition to transition metal compounds with carbene and oxo groups LnM(η ³ CH ₂)(η ³ O). Journal of Physical Organic Chemistry, 2007, 20, 11-18. | 0.9 | 18 |
| 3258 | Evaluation of various DFT protocols for computing ¹ H and ¹³ C chemical shifts to distinguish stereoisomers: diastereomeric 2-, 3-, and 4-methylcyclohexanols as a test set. Journal of Physical Organic Chemistry, 2007, 20, 345-354. | 0.9 | 26 |
| 3259 | Brother versus brother: competitive stabilization of carbocationic centers by flanking cyclopropanes and i ⁺ -systems. Journal of Physical Organic Chemistry, 2007, 20, 384-394. | 0.9 | 10 |
| 3260 | Physical image vs structure relation: part 12 - structure of 2,2,5,5-tetramethyl-dihydro-furan-3-one oxime and its protonated forms through isomerization and NMR spectra. Journal of Physical Organic Chemistry, 2007, 20, 422-430. | 0.9 | 8 |
| 3261 | Synthesis and structural study of 2- and 2,6- positioned methyl- and nitro- substituted 3-(arylhydrazono)pentane-2,4-diones. Journal of Physical Organic Chemistry, 2007, 20, 716-731. | 0.9 | 29 |
| 3262 | Ice nanoclusters at hydrophobic metal surfaces. Nature Materials, 2007, 6, 597-601. | 13.3 | 303 |
| 3263 | Quantum DFT and DF-DFT study of vibrational spectra of sulfuric acid, sulfuric acid monohydrate, formic acid and its cyclic dimer. Vibrational Spectroscopy, 2007, 44, 286-296. | 1.2 | 28 |
| 3264 | Chemistry of naphthazarine derivatives: XIV. Preparative synthesis of 1-bromoalkylnaphthazarines. Russian Journal of Organic Chemistry, 2007, 43, 1170-1175. | 0.3 | 4 |
| 3265 | Oligothiophene- and Oligopyrrole-Mediated Aggregation of Gold Nanoparticles. Journal of Physical Chemistry C, 2007, 111, 5886-5892. | 1.5 | 18 |
| 3266 | Computing Reliable Energetics for Conjugate Addition Reactions. Organic Letters, 2007, 9, 4279-4282. | 2.4 | 67 |
| 3267 | Critical analysis of the local aromaticity concept in polyaromatic hydrocarbons. Faraday Discussions, 2007, 135, 347-365. | 1.6 | 156 |
| 3268 | Local Modifications of Single-Wall Carbon Nanotubes Induced by Bond Formation with Encapsulated Fullerenes. Journal of Physical Chemistry B, 2007, 111, 1099-1109. | 1.2 | 32 |
| 3269 | Prediction of the vapor pressure and vaporization enthalpy of 1-n-alkyl-3-methylimidazolium-bis-(trifluoromethanesulfonyl) amide ionic liquids. Physical Chemistry Chemical Physics, 2007, 9, 4653. | 1.3 | 79 |
| 3270 | On the Theory of Organic Catalysis on Water. Journal of the American Chemical Society, 2007, 129, 5492-5502. | 6.6 | 587 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3271 | Generation of Free Radicals by Emodic Acid and its [d-Lys6]GnRH-conjugate. Photochemistry and Photobiology, 2007, 74, 226-236. | 1.3 | 1 |
| 3272 | On the Formation of Cyclobutane Pyrimidine Dimers in UV-irradiated DNA: Why are Thymines More Reactive? Photochemistry and Photobiology, 2007, 78, 159-167. | 1.3 | 5 |
| 3273 | Mechanism of Thermal Unimolecular Decomposition of TNT (2,4,6-Trinitrotoluene): A DFT Study. Journal of Physical Chemistry A, 2007, 111, 11074-11083. | 1.1 | 111 |
| 3275 | Theoretical modeling of spectroscopic properties of molecules in solution: toward an effective dynamical discrete/continuum approach. Theoretical Chemistry Accounts, 2007, 117, 1001-1015. | 0.5 | 59 |
| 3276 | Reparameterization of a meta-generalized gradient approximation functional by combining TPSS exchange with $\tilde{\tau}$,1 correlation. Theoretical Chemistry Accounts, 2007, 118, 693-707. | 0.5 | 19 |
| 3277 | Gradient incorporation in one-dimensional applications of interpolating moving least-squares methods for fitting potential energy surfaces. Theoretical Chemistry Accounts, 2007, 118, 755-767. | 0.5 | 11 |
| 3278 | Raman spectroscopic investigation of the antimalarial agent mefloquine. Analytical and Bioanalytical Chemistry, 2007, 387, 1749-1757. | 1.9 | 41 |
| 3279 | Piperidine adsorption on two different silver electrodes: A combined surface enhanced Raman spectroscopy and density functional theory study. Journal of Nanoparticle Research, 2007, 9, 817-824. | 0.8 | 11 |
| 3280 | Performance of theoretical methods and basis sets on the molecular structure, atomisation and ionisation energies, electron affinity, and vibrational spectrum of silylene. Silicon Chemistry, 2007, 3, 251-257. | 0.8 | 2 |
| 3281 | Ligand Exchange Processes on Solvated Lithium Cations. II. Complexation by Cryptands in β -Butyrolactone as Solvent. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2007, 58, 81-88. | 1.6 | 11 |
| 3282 | Structural Analysis of Bisphenol-A and its Methylene, Sulfur, and Oxygen Bridged Bisphenol Analogs. Journal of Chemical Crystallography, 2007, 37, 587-595. | 0.5 | 18 |
| 3283 | Non-empirical investigation of the geometrical structure and energy stability of dimers of yttrium β -diketonates Y2(MDA)6 and Y2(HFA)6. Journal of Structural Chemistry, 2007, 48, 796-810. | 0.3 | 4 |
| 3284 | Hybrid exchange correlation functionals and potentials: Concept elaboration. Journal of Structural Chemistry, 2007, 48, S1-S31. | 0.3 | 40 |
| 3285 | Computational modeling of factors that modulate the unique FeNO bonding in {FeNO}6 heme-thiolate model complexes. Journal of Biological Inorganic Chemistry, 2007, 12, 721-731. | 1.1 | 6 |
| 3286 | Kinetics and mechanism of the substitution reactions of [PtCl(bpma)]+, [PtCl(gly-met-S,N,N)] and their aqua analogues with l-methionine, glutathione and 5'-GMP. Journal of Biological Inorganic Chemistry, 2007, 12, 1141-1150. | 1.1 | 36 |
| 3287 | Theoretical investigation on the oxidative chlorination performed by a biomimetic non-heme iron catalyst. Journal of Biological Inorganic Chemistry, 2007, 12, 1151-1162. | 1.1 | 27 |
| 3288 | Validation of density functional modeling protocols on experimental bis(μ -4-oxo)/ μ -4- $\hat{1}$:2- $\hat{1}$:2-peroxo dicopper equilibria. Journal of Biological Inorganic Chemistry, 2007, 12, 1221-1234. | 1.1 | 35 |
| 3289 | Multipole electrostatic potential derived atomic charges in NDDO-methods with spd-basis sets. Journal of Molecular Modeling, 2007, 13, 381-392. | 0.8 | 2 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3290 | Density functional study of isoguanine tetrad and pentad sandwich complexes with alkali metal ions. <i>Journal of Molecular Modeling</i> , 2007, 13, 335-345. | 0.8 | 17 |
| 3291 | Calculations of the C2 fragmentation energies of higher fullerenes C80 and C82. <i>Journal of Molecular Modeling</i> , 2007, 13, 981-986. | 0.8 | 2 |
| 3292 | A comparison of transition state of phenol in H-atom abstraction by methyl and methylperoxyl radicals. <i>Science Bulletin</i> , 2007, 52, 1182-1186. | 1.7 | 2 |
| 3293 | Gas-phase ion chemistry of NF ₃ /SO ₂ mixtures: A mass spectrometric and theoretical investigation. <i>International Journal of Mass Spectrometry</i> , 2007, 266, 86-91. | 0.7 | 2 |
| 3294 | Theoretical studies on the electronic structures and optical properties of the oligomers involving bipyridyl, thiophenyl and ethynyl groups. <i>Polymer</i> , 2007, 48, 502-511. | 1.8 | 40 |
| 3295 | Highly stereoselective and easy synthesis of enantiopure phosphoranyl oxiranes. <i>Tetrahedron: Asymmetry</i> , 2007, 18, 2617-2620. | 1.8 | 9 |
| 3296 | Insights into the nature of the hydrogen bonding of Tyr272 in apo-galactose oxidase. <i>Journal of Inorganic Biochemistry</i> , 2007, 101, 1859-1864. | 1.5 | 9 |
| 3297 | Cytotoxic studies of substituted titanocene and ansa-titanocene anticancer drugs. <i>Journal of Inorganic Biochemistry</i> , 2008, 102, 1558-1570. | 1.5 | 59 |
| 3298 | The photophysics of 7H-adenine: A quantum chemical investigation including spin-orbit effects. <i>Chemical Physics</i> , 2008, 347, 346-359. | 0.9 | 23 |
| 3299 | The use of Coulomb-attenuated methods for the calculation of electronic circular dichroism spectra. <i>Chemical Physics</i> , 2008, 349, 234-243. | 0.9 | 39 |
| 3300 | Theoretical studies of the electronic structures and optical properties of stable blue-emitting polymer based on 4H-cyclopenta-[def]-phenanthrene. <i>Polymer</i> , 2008, 49, 2077-2084. | 1.8 | 5 |
| 3301 | Understanding the π -facial diastereoselectivity in the addition of chiral diaminophosphino(silyl)carbenes to activated olefins. <i>Tetrahedron: Asymmetry</i> , 2008, 19, 2353-2358. | 1.8 | 7 |
| 3302 | A DFT study on secondary reaction pathways in the acid-catalysed Beckmann rearrangement of cyclohexanone oxime in aprotic solvent. <i>Computational and Theoretical Chemistry</i> , 2008, 858, 46-51. | 1.5 | 25 |
| 3303 | Application of Density Functional Theory for evaluation of standard two-electron reduction potentials in some quinone derivatives. <i>Computational and Theoretical Chemistry</i> , 2008, 870, 10-14. | 1.5 | 16 |
| 3304 | Reduction of N ₂ by Fe ²⁺ via Homogeneous and Heterogeneous Reactions Part 2: The Role of Metal Binding in Activating N ₂ for Reduction; a Requirement for Both Pre-biotic and Biological Mechanisms. <i>Origins of Life and Evolution of Biospheres</i> , 2008, 38, 195-209. | 0.8 | 10 |
| 3305 | Conformational analysis and interpretation of $\hat{\nu}_{1/2}(\text{OH})$ band in the IR spectrum of o-vinylphenol: a DFT study. <i>Russian Chemical Bulletin</i> , 2008, 57, 510-519. | 0.4 | 3 |
| 3306 | Coordination chemistry of anticrowns. Complexation of cyclic trimeric perfluoro-o-phenylenemercury (o-C ₆ F ₄ Hg) ₃ with the cyanoborohydride anion [H ₃ BCN] ⁻ and triethylamineborane Et ₃ NBH ₃ . <i>Russian Chemical Bulletin</i> , 2008, 57, 2540-2547. | 0.4 | 7 |
| 3307 | Synthesis, X-ray crystallography characterization, vibrational spectroscopy, and DFT theoretical studies of a new organic-inorganic hybrid material. <i>Structural Chemistry</i> , 2008, 19, 155-164. | 1.0 | 16 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3308 | Crystallographic and conformational analysis of (E)-2-isopropyl-4-(p-tolyldiazenyl)phenol. <i>Structural Chemistry</i> , 2008, 19, 565-570. | 1.0 | 5 |
| 3309 | Ab initio and DFT theory studies of interaction of thymine with formaldehyde. <i>Structural Chemistry</i> , 2008, 19, 843-847. | 1.0 | 8 |
| 3310 | Desynchronization of Pedal Motion: Crystallographic and Theoretical Study of (E)-4-[(4-ethylphenyl)diazenyl]-2-methylphenol. <i>Journal of Chemical Crystallography</i> , 2008, 38, 671-677. | 0.5 | 4 |
| 3311 | Statistical spectroscopy as a tool for the study of molecular similarity. <i>Journal of Mathematical Chemistry</i> , 2008, 43, 1560-1572. | 0.7 | 11 |
| 3312 | Camphor-based $\hat{\pm}$ -bromoketones for the asymmetric darzens reaction: Insights into the mechanism using density functional theory. <i>Journal of Structural Chemistry</i> , 2008, 49, 818-827. | 0.3 | 2 |
| 3313 | Study of the structural and thermodynamic stability of pentacoordinated nitrogen compounds NF ₂ X ₃ (X = H, Cl, Br): Ab initio calculations. <i>Journal of Structural Chemistry</i> , 2008, 49, 973-978. | 0.3 | 7 |
| 3314 | Quadrupole coupling constants and isomeric Mössbauer shifts for halogen-containing gold, platinum, niobium, tantalum and antimony compounds. <i>Hyperfine Interactions</i> , 2008, 181, 27-36. | 0.2 | 4 |
| 3315 | Host-guest complexes of mixed glycol-phenanthroline cryptands: prediction of ion selectivity by quantum chemical calculations IV. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2008, 60, 383-392. | 1.6 | 15 |
| 3316 | Characterizing vibrational motion beyond internal coordinates. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 113-131. | 0.5 | 39 |
| 3317 | Philip J. Stephens: A scientific memoir. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 5-18. | 0.5 | 6 |
| 3318 | A vibrational circular dichroism implementation within a Slater-type-orbital based density functional framework and its application to hexa- and hepta-helicenes. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 245-263. | 0.5 | 87 |
| 3319 | An IEF-PCM study of solvent effects on the Faraday B term of MCD. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 231-244. | 0.5 | 31 |
| 3320 | Determination of the absolute configuration of chiral molecules via density functional theory calculations of vibrational circular dichroism and optical rotation: The chiral alkane D3-anti-trans-anti-trans-anti-trans-perhydrotriphenylene. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 19-28. | 0.5 | 25 |
| 3321 | A liposomal dispersion formulation of propofol: formulation, pharmacokinetics, stability, and identification of an oxidative degradant. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 291-296. | 0.5 | 3 |
| 3322 | Anharmonic vibrational spectroscopy calculations with electronic structure potentials: comparison of MP2 and DFT for organic molecules. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 273-279. | 0.5 | 51 |
| 3323 | The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 215-241. | 0.5 | 23,928 |
| 3324 | Current-voltage curves for molecular junctions: the issue of the basis set for the metal contacts. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 429-435. | 0.5 | 5 |
| 3325 | Car-Parrinello molecular dynamics simulations and EPR property calculations on aqueous ubisemiquinone radical anion. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 477-487. | 0.5 | 28 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3326 | Theoretical design of blue emitting materials based on symmetric and asymmetric spiro-silabifluorene derivatives. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 489-500. | 0.5 | 12 |
| 3327 | Structure and electron paramagnetic resonance parameters of the manganese site of concanavalin A studied by density functional methods. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 437-445. | 0.5 | 7 |
| 3328 | Theoretical study of the gas-phase ethane C-H and C-C bonds activation by bare niobium cation. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 395-403. | 0.5 | 9 |
| 3329 | On the TD-DFT UV/vis spectra accuracy: the azoalkanes. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 405-410. | 0.5 | 56 |
| 3330 | Theoretical modeling of open-shell molecules in solution: a QM/MM molecular dynamics approach. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 499-506. | 0.5 | 7 |
| 3331 | Effect of molecular size on the parity-non-conserving contributions to the nuclear magnetic resonance shielding constant. <i>Theoretical Chemistry Accounts</i> , 2008, 121, 53-57. | 0.5 | 5 |
| 3332 | Azobenzene-functionalized alkanethiols in self-assembled monolayers on gold. <i>Applied Physics A: Materials Science and Processing</i> , 2008, 93, 267-275. | 1.1 | 35 |
| 3333 | Theoretical study on the reaction mechanism of CN radical with ketene. <i>Science in China Series B: Chemistry</i> , 2008, 51, 101-110. | 0.8 | 3 |
| 3334 | Spin-state-dependent oxygen sensitivity of iron dithiolates: sulfur oxygenation or disulfide formation. <i>Journal of Biological Inorganic Chemistry</i> , 2008, 13, 1219-1230. | 1.1 | 28 |
| 3335 | DFT-based molecular modeling and vibrational study of the La(III) complex of 3,3'-bis(benzylidene)bis(4-hydroxycoumarin). <i>Journal of Molecular Modeling</i> , 2008, 14, 353-366. | 0.8 | 33 |
| 3336 | ParaFrag—an approach for surface-based similarity comparison of molecular fragments. <i>Journal of Molecular Modeling</i> , 2008, 14, 547-558. | 0.8 | 19 |
| 3337 | Theoretical and experimental study of molecular structure and vibrational spectra of N-(2-pyridylmethyl)-2-pyrazinecarboxamide. <i>Monatshefte für Chemie</i> , 2008, 139, 773-780. | 0.9 | 19 |
| 3338 | N-Methyl-N-phenylaminomethyl 2-naphthyl ketone: an X-ray diffraction and density functional theory study. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2008, 64, o155-o158. | 0.4 | 1 |
| 3339 | Theoretical prediction of linear free energy relationships using proton nucleomers. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 136-145. | 0.9 | 5 |
| 3340 | Feasibility of the spontaneous gas-phase proton transfer equilibria between neutral Brønsted acids and Brønsted bases. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 571-574. | 0.9 | 10 |
| 3341 | Structural aspects of the intermolecular hydrogen bond strength: H-bonded complexes of aniline, phenol and pyridine derivatives. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 897-914. | 0.9 | 80 |
| 3342 | Structure and stability of B ₅ C and C ₅ B clusters. <i>Rapid Communications in Mass Spectrometry</i> , 2008, 22, 3599-3607. | 0.7 | 10 |
| 3343 | A comparative DFT study of substrates and products of industrial enzyme nitrile hydratase. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 161-179. | 1.0 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3344 | Poor enantioselectivity of the direct aldol reaction catalyzed by (S,S)-proline dipeptide: A density functional study. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 66-74. | 1.0 | 2 |
| 3345 | Performance of DFT hybrid functionals in the theoretical treatment of Hâ€bonds: Analysis termâ€byâ€term. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 229-237. | 1.0 | 13 |
| 3346 | Conformational analysis of cycloheptane, oxacycloheptane, 1,2â€dioxacycloheptane, 1,3â€dioxacycloheptane, and 1,4â€dioxacycloheptane. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 339-350. | 1.0 | 26 |
| 3347 | Stability, structural properties, and dissociation pathways of silylidyneâ€amines RSiN and silylidyneâ€phosphanes RSiP (R = F, Cl). <i>International Journal of Quantum Chemistry</i> , 2008, 108, 447-455. | 1.0 | 7 |
| 3348 | Solvent effect of aqueous media on properties of glycine: Significance of specific and bulk solvent effects, and geometry optimization in aqueous media. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1004-1016. | 1.0 | 27 |
| 3349 | Structural studies of the water tetramer. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1653-1659. | 1.0 | 105 |
| 3350 | Effects of methods and basis set on ab initio calculations of electronic transport through hydrogenated Pt nanocontacts. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1637-1644. | 1.0 | 6 |
| 3351 | Quantum mechanical model for Maya Blue. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1664-1673. | 1.0 | 29 |
| 3352 | Electronic structure of CuX^{<i>y</i>} (X = B, C, N, O, F; <i>y</i> = 0, +1, â³1). <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2512-2522. | 1.0 | 7 |
| 3353 | A DFT study of infrared spectrum of sphingomyelin lipid molecule with calcium cation. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2935-2942. | 1.0 | 7 |
| 3354 | Novel effects in finiteâ€length silicon nanowires. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2008, 205, 2625-2629. | 0.8 | 2 |
| 3355 | Exciting prospects for solids: Exactâ€exchange based functionals meet quasiparticle energy calculations. <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 929-945. | 0.7 | 83 |
| 3356 | Interannular Nitrogenâ€Lithium Bridges in Ferrocenophanes. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2008, 634, 311-316. | 0.6 | 3 |
| 3357 | Ligand Exchange Processes on Solvated Beryllium Cations. II [Be(solvent)(12â€Crownâ€4)]²⁺. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2008, 634, 735-739. | 0.6 | 28 |
| 3358 | Ferrocene Derivatives Bearing one and two Isocyanato, Isothiocyanato and Isoselenocyanato Substituents. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2008, 634, 1434-1438. | 0.6 | 6 |
| 3359 | Die Kristallstruktur von [BeCl2(15-Krone-5)]. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2008, 634, 1473-1476. | 0.6 | 32 |
| 3360 | Ethylene Addition to Groupâ€9 Transition Metal Dioxo Compounds â€ A Quantum Chemical Study. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2008, 634, 2145-2155. | 0.6 | 9 |
| 3361 | Ligand Exchange Processes on Solvated Beryllium Cations. IV <i>Anorganische Und Allgemeine Chemie</i> , 2008, 634, 1915-1920. | 0.6 | 16 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3362 | Complete basis set B3LYP NMR calculations of CDCl ₃ solvent's water fine spectral details. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, 851-858. | 1.1 | 31 |
| 3363 | ⁵⁷ Fe NMR spectroscopy of ferrocenes derived from aminoferrocene and 1,1- ² -diaminoferrrocene. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, S30-S35. | 1.1 | 12 |
| 3364 | The electronic delocalization in <i>para</i> -substituted ¹³ C-nitrostyrenes probed by resonance Raman spectroscopy and quantum ² calculations. <i>Journal of Raman Spectroscopy</i> , 2008, 39, 453-459. | 1.2 | 7 |
| 3365 | Thermal decomposition reaction and a comprehensive kinetic model of dimethyl ether. <i>International Journal of Chemical Kinetics</i> , 2008, 40, 1-18. | 1.0 | 411 |
| 3366 | The Rate-Determining Step in the Rhodium-Xantphos-Catalysed Hydroformylation of 1-Octene. <i>Chemistry - A European Journal</i> , 2008, 14, 1843-1853. | 1.7 | 75 |
| 3367 | Palladium-Catalysed [3+2] Cycloaddition of Alk-5-ynylidenecyclopropanes to Alkynes: A Mechanistic DFT Study. <i>Chemistry - A European Journal</i> , 2008, 14, 272-281. | 1.7 | 45 |
| 3368 | Octahedral Adducts of Dichlorosilane with Substituted Pyridines: Synthesis, Reactivity and a Comparison of Their Structures and ²⁹ Si-NMR Chemical Shifts. <i>Chemistry - A European Journal</i> , 2008, 14, 3164-3176. | 1.7 | 38 |
| 3369 | Density Functional Theory Study of <i>trans</i> -Dioxo Complexes of Iron, Ruthenium, and Osmium with Saturated Amine Ligands, <i>trans</i> -[M(O) ₂ (NH) ₃] ₂ (NMeH) ₂ (M=Fe, Ru, Os), and Detection of [Fe(qpy)(O) ₂] _n (n=1, 2) by High-Resolution ESI Mass Spectrometry. <i>Chemistry - A European Journal</i> , 2008, 14, 5495-5506. | 1.7 | 13 |
| 3370 | Polyhedral Structures with Three-, Four-, and Five Fold Symmetry in Metal-Centered Ten-Vertex Germanium Clusters. <i>Chemistry - A European Journal</i> , 2008, 14, 4542-4550. | 1.7 | 20 |
| 3371 | Mechanism of the Rhodium-Catalyzed Asymmetric Isomerization of Allylamines to Enamines. <i>Chemistry - A European Journal</i> , 2008, 14, 3323-3329. | 1.7 | 17 |
| 3372 | Why do Cationic Hydrido-iridium(III) Complexes with ² Aminophosphane Ligands Favour the Transfer Hydrogenation of Ketones over the Direct ² Hydrogenation? A Computational Approach. <i>Chemistry - A European Journal</i> , 2008, 14, 8898-8903. | 1.7 | 19 |
| 3373 | New Rare Earth Metal Complexes with Nitrogen-Rich Ligands: 5,5-Bitetrazolate and 1,3-Bis(tetrazol-5-yl)triazene. On the Borderline between Coordination and the Formation of Salt-Like Compounds. <i>Chemistry - A European Journal</i> , 2008, 14, 3727-3736. | 1.7 | 41 |
| 3374 | The Phenoxy/Phenol/Copper Cation: A Minimalistic Model of Bonding Relations in Active Centers of Mononuclear Copper Enzymes. <i>Chemistry - A European Journal</i> , 2008, 14, 4318-4327. | 1.7 | 64 |
| 3375 | On the Mechanism of the Thermal Retrocycloaddition of Pyrrolidinofullerenes (Retro-Prato) Tj ETQq1 1 0.784314 rgBT / Overlock 10 | 1.7 | 56 |
| 3376 | Mono- and Diprotonation of the Superbasic Bisguanidine 1,2-Bis(<i>N,N,N</i> -(² tetramethylguanidino)benzene (btmgb) and Pt ^{II} and Pt ^{IV} Complexes of Chelating Bisguanidines and Guanidates. <i>Chemistry - A European Journal</i> , 2008, 14, 7813-7821. | 1.7 | 49 |
| 3377 | The Elusive Structure of CrCl ₂ : A Combined Computational and Gas-Phase Electron-Diffraction Study. <i>Chemistry - A European Journal</i> , 2008, 14, 5130-5143. | 1.7 | 20 |
| 3378 | Helicate Extension as a Route to Molecular Wires. <i>Chemistry - A European Journal</i> , 2008, 14, 7180-7185. | 1.7 | 32 |
| 3379 | Mechanisms of Air Oxidation of Ethoxylated Surfactants: Computational Estimations of Energies and Reaction Behaviors. <i>Chemistry - A European Journal</i> , 2008, 14, 9549-9554. | 1.7 | 8 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3380 | Characterization of Three Members of the Electron Transfer Series [Fe(pda) ₂] ^(i>n</i>=2⁺, 1⁺, 0) by Spectroscopy and Density Functional Theoretical Calculations [pda=Redox Noninnocent Derivatives of <i>N,N</i> -bis(pentafluorophenyl)phenylenediamide(2 ⁺ , 1 ⁺ , 0)]. Chemistry - A European Journal, 2008, 14, 7608-7622. | 1.7 | 44 |
| 3381 | Construction of Titanasiloxanes by Incorporation of Silanols to the Metal Oxide Model [{Ti(⁵ Me) ₅ (^{1/4} O)} ₃ (³ CR)]: DFT Elucidation of the Reaction Mechanism. Chemistry - A European Journal, 2008, 14, 7930-7938. | | 20 |
| 3382 | Models of the ox1 State of Methylcoenzyme M Reductase: Where are the Electrons?. Chemistry - A European Journal, 2008, 14, 9981-9989. | 1.7 | 3 |
| 3383 | Aromatic Hydroxylation in a Copper Bis(imine) Complex Mediated by a ^{1/4} · ¹ · Peroxo Dicopper Core: A Mechanistic Scenario. Chemistry - A European Journal, 2008, 14, 9714-9729. | 1.7 | 52 |
| 3384 | Aldol Reactions between <i>L</i> -Erythrulose Derivatives and Chiral \pm -Amino and \pm -Fluoro Aldehydes: Competition between Felkin-Anh and Cornforth Transition States. Chemistry - A European Journal, 2008, 14, 9240-9254. | 1.7 | 20 |
| 3385 | Effect of the Nature of the Metal Atom on Hydrogen Bonding and Proton Transfer to [Cp* <i>M</i> H ₃ (dppe)]: Tungsten versus Molybdenum. Chemistry - A European Journal, 2008, 14, 9921-9934. | 1.7 | 28 |
| 3386 | Living Radical Polymerization of Acrylates Mediated by 1,3-Bis(2-pyridylimino)isoindolatocobalt(II) Complexes: Monitoring the Chain Growth at the Metal. Chemistry - A European Journal, 2008, 14, 10267-10279. | 1.7 | 70 |
| 3387 | Stereoselective Alcohol Silylation by Dehydrogenative Si-O Coupling: Scope, Limitations, and Mechanism of the Cu-H-Catalyzed Nonenzymatic Kinetic Resolution with Silicon Stereogenic Silanes. Chemistry - A European Journal, 2008, 14, 11512-11528. | 1.7 | 84 |
| 3388 | Measured and calculated CD spectra of G-quartets stacked with the same or opposite polarities. Chirality, 2008, 20, 431-440. | 1.3 | 202 |
| 3389 | The determination of the absolute configurations of chiral molecules using vibrational circular dichroism (VCD) spectroscopy. Chirality, 2008, 20, 643-663. | 1.3 | 323 |
| 3390 | 6-Thioguanine in DNA as CD spectroscopic probe to study local structural changes upon protein binding. Chirality, 2008, 20, 978-984. | 1.3 | 8 |
| 3391 | Static and Frequency-Dependent Dipole-Dipole Polarizabilities of All Closed-Shell Atoms up to Radium: A Four-Component Relativistic DFT Study. ChemPhysChem, 2008, 9, 445-453. | 1.0 | 27 |
| 3392 | Thin-Film Properties of DNA and RNA Bases: A Combined Experimental and Theoretical Study. ChemPhysChem, 2008, 9, 740-747. | 1.0 | 27 |
| 3393 | Understanding the Supramolecular Self-Assembly of the Fullerene Derivative PCBM on Gold Surfaces. ChemPhysChem, 2008, 9, 1030-1035. | 1.0 | 21 |
| 3394 | Selective Homogeneous and Heterogeneous Gold Catalysis with Alkynes and Alkenes: Similar Behavior, Different Origin. ChemPhysChem, 2008, 9, 1624-1629. | 1.0 | 119 |
| 3395 | IR, Raman, and UV/Vis Spectra of Corannulene for Use in Possible Interstellar Identification. ChemPhysChem, 2008, 9, 2085-2091. | 1.0 | 33 |
| 3396 | Structural Characteristics of Hydrogenated Carbon and Boron Nitride Nanotubes: Impact of H ₂ /H Interactions. ChemPhysChem, 2008, 9, 2390-2396. | 1.0 | 9 |
| 3397 | A DFT-Based Investigation of Hydrogen Abstraction Reactions from Methylated Polycyclic Aromatic Hydrocarbons. ChemPhysChem, 2008, 9, 2349-2358. | 1.0 | 27 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3398 | Ligand Exchange Processes on Solvated Beryllium Cations. Part III. Helvetica Chimica Acta, 2008, 91, 1063-1071. | 1.0 | 24 |
| 3399 | Benchmarking approximate density functional theory for s/d excitation energies in 3d transition metal cations. Journal of Computational Chemistry, 2008, 29, 185-189. | 1.5 | 61 |
| 3400 | Calculation of weakly polar interaction energies in polypeptides using density functional and local Møller-Plesset perturbation theory. Journal of Computational Chemistry, 2008, 29, 1344-1352. | 1.5 | 30 |
| 3401 | On the performance of some aromaticity indices: A critical assessment using a test set. Journal of Computational Chemistry, 2008, 29, 1543-1554. | 1.5 | 261 |
| 3402 | Basis set dependence of solute-solvent interaction energy of benzene in water: A HF/DFT study. Journal of Computational Chemistry, 2008, 29, 1725-1732. | 1.5 | 8 |
| 3403 | Synthesis and Structural Characterisation of cis- and trans-[(hppH)2PtCl2], [(hppH)3PtCl]+ Cl- and Some New Salts of the [hppH2]+ Cation (hppH = 1,3,4,6,7,8-Hexahydro-2H-pyrimido[1,2-a]pyrimidine): The Importance of Hydrogen Bonding. European Journal of Inorganic Chemistry, 2008, 2008, 1248-1257. | 1.0 | 30 |
| 3404 | Ruthenium Dihydrogen Complex for C-H Activation: Catalytic H/D Exchange under Mild Conditions. European Journal of Inorganic Chemistry, 2008, 2008, 3493-3500. | 1.0 | 39 |
| 3405 | Beyond the Icosahedron: A Density Functional Theory Study of 14-Atom Germanium Clusters. European Journal of Inorganic Chemistry, 2008, 2008, 3996-4003. | 1.0 | 11 |
| 3406 | Mechanistic Insights into Acetophenone Transfer Hydrogenation Catalyzed by Half-Sandwich Ruthenium(II) Complexes Containing 2-(Diphenylphosphanyl)aniline - A Combined Experimental and Theoretical Study. European Journal of Inorganic Chemistry, 2008, 2008, 4462-4473. | 1.0 | 45 |
| 3407 | The First Metal Complexes of the Proton Sponge 1,8-Bis(N,N-dimethyltetramethylguanidino)naphthalene: Syntheses and Properties. European Journal of Inorganic Chemistry, 2008, 2008, 4440-4447. | 1.0 | 41 |
| 3408 | A Proton-Triggered Cascade Reaction Involving a Heavy p-Block Multiple Bond: Transformation of the Diphosphene C5Me5P=PC5Me5 into the Cationic Cage [C10Me10P2H]+. European Journal of Inorganic Chemistry, 2008, 2008, 4511-4515. | 1.0 | 9 |
| 3409 | Serinic Aminoacrylates: Iterative Synthesis of N-Substituted Amino-1,3-dioxane Derivatives from N-(p-Nitrophenyl)serinols and Rotational Stereochemistry Phenomena. European Journal of Organic Chemistry, 2008, 2008, 2473-2494. | 1.2 | 11 |
| 3410 | 1,6-Electrocyclization of Azatriene Derivatives. European Journal of Organic Chemistry, 2008, 2008, 1092-1100. | 1.2 | 18 |
| 3411 | Synthesis and Characterization of Cyclopropylpolyketides: A Combined Experimental and Theoretical Study. European Journal of Organic Chemistry, 2008, 2008, 971-974. | 1.2 | 3 |
| 3412 | DFT Study of Brønsted Acid Catalyzed Nitroso Aldol Reaction Between Achiral Enamines and Nitrosobenzene: The Reason for Regio- and Enantioselectivity. European Journal of Organic Chemistry, 2008, 2008, 4245-4249. | 1.2 | 14 |
| 3413 | The Mechanism of the Stetter Reaction - A DFT Study. European Journal of Organic Chemistry, 2008, 2008, 5563-5570. | 1.2 | 91 |
| 3414 | Theoretical Description of Substituent Effects in Electrophilic Aromatic Substitution Reactions. European Journal of Organic Chemistry, 2008, 2008, 5928-5935. | 1.2 | 10 |
| 3415 | DFT/MM Study on Copper-Catalyzed Cyclopropanation - Enantioselectivity with No Enthalpy Barrier. European Journal of Organic Chemistry, 2008, 2008, 5614-5621. | 1.2 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3416 | 1,2,4,5-tetrakis(tetramethylguanidino)benzene: Synthesis and Properties of a New Molecular Electron Donor. <i>European Journal of Organic Chemistry</i> , 2008, 2008, 5907-5914. | 1.2 | 91 |
| 3417 | CYP17 Inhibitors. Annulations of Additional Rings in Methylene Imidazole Substituted Biphenyls: Synthesis, Biological Evaluation and Molecular Modelling. <i>Archiv Der Pharmazie</i> , 2008, 341, 597-609. | 2.1 | 24 |
| 3418 | A Polar Radical Pair Pathway To Assemble the Pyrimidinone Core of the HIV Integrase Inhibitor Raltegravir Potassium. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 4134-4136. | 7.2 | 25 |
| 3419 | Multiply Charged (Di)Radicals. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 151-154. | 7.2 | 23 |
| 3420 | A General Strategy for Construction of Both 2,6-cis- and 2,6-trans-Disubstituted Tetrahydropyrans: Substrate-Controlled Asymmetric Total Synthesis of (+)-Scanlonenyne. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 4200-4203. | 7.2 | 37 |
| 3421 | Pronounced Steric Effects of Substituents in the Nazarov Cyclization of Aryl Dienyl Ketones. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 6379-6383. | 7.2 | 67 |
| 3422 | Sources of Error in DFT Computations of C≡C Bond Formation Thermochemistries: $\ddot{\text{C}}\text{C}^{\ddagger}\text{f}$ Transformations and Error Cancellation by DFT Methods. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 7746-7749. | 7.2 | 162 |
| 3423 | Gas-Phase Formation of the Gomberg-Bachmann Magnesium Ketyl. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 9118-9121. | 7.2 | 38 |
| 3424 | $\text{Bi}(\text{OTf})_3$ -Catalyzed Diastereoselective $\text{S}_{\text{N}}1$ -Type Reactions of Chiral Propargylic Acetates. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 10106-10109. | 7.2 | 58 |
| 3425 | Synthesis and structure of novel spirosilanes. Combination of 1,2-hydroboration and 1,1-organoboration. <i>Applied Organometallic Chemistry</i> , 2008, 22, 383-388. | 1.7 | 27 |
| 3433 | Comparative studies on adsorption behavior of thionine on gold nanoparticles with different sizes. <i>Journal of Colloid and Interface Science</i> , 2008, 327, 243-250. | 5.0 | 36 |
| 3434 | Growth mechanism of catalyst- and template-free group III-nitride nanorods. <i>Journal of Crystal Growth</i> , 2008, 310, 3735-3740. | 0.7 | 14 |
| 3435 | An experimental and theoretical study of molecular structure and vibrational spectra of pentafluorophenylboronic acid molecule by density functional theory and ab initio Hartree Fock calculations. <i>Journal of Molecular Structure</i> , 2008, 874, 159-169. | 1.8 | 29 |
| 3436 | Infrared spectrum and STM images of cyclohexene-2-ethanamine: First principle investigation. <i>Journal of Molecular Structure</i> , 2008, 886, 144-147. | 1.8 | 0 |
| 3437 | Polyamines. Part II: Spectroscopic properties of N,N-dimethyl-3-phthalimidopropylammonium acetate and hydrochloride and supramolecular interactions in their crystals. <i>Journal of Molecular Structure</i> , 2008, 891, 205-213. | 1.8 | 4 |
| 3438 | Computational studies of CO and CO ⁺ : Density functional theory and time-dependent density functional theory. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2008, 109, 2546-2560. | 1.1 | 9 |
| 3439 | Quantum chemical study and low-temperature calorimetry of phase transition in V ₄ S ₉ Br ₄ . <i>Journal of Solid State Chemistry</i> , 2008, 181, 2877-2881. | 1.4 | 6 |
| 3440 | Structural study of 2-(1-oxo-1 H-inden-3-yl)-2H-indene-1,3-dione by DFT calculations, NMR and IR spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 70, 94-98. | 2.0 | 45 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3441 | An experimental and theoretical study of molecular structure and vibrational spectra of 3- and 4-pyridineboronic acid molecules by density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 70, 664-673. | 2.0 | 77 |
| 3442 | The most stable tautomer of 3-amino-1,2,4-triazin-5-one and its structural geometry. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 70, 1020-1024. | 2.0 | 2 |
| 3443 | Comparison of experimental and density functional study on the molecular structure, infrared and Raman spectra and vibrational assignments of 6-chloronicotinic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 876-883. | 2.0 | 74 |
| 3444 | FT-IR, FT-Raman spectra and ab initio HF and DFT calculations of 4-N,N ² -dimethylamino pyridine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 898-906. | 2.0 | 144 |
| 3445 | Theoretical investigation of the molecular, electronic structures and vibrational spectra of a series of first transition metal phthalocyanines by Z. Liu et al.. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 286-287. | 2.0 | 18 |
| 3446 | Molecular structure and vibrational spectra of 3-chloro-4-fluoro benzonitrile by ab initio HF and density functional method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 1134-1139. | 2.0 | 80 |
| 3447 | Vibrational spectroscopy of triacetone triperoxide (TATP): Anharmonic fundamentals, overtones and combination bands. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 1438-1445. | 2.0 | 30 |
| 3448 | Quantum chemical study of the intermediate complex required for iron-mediated reactivity and antimalarial activity of dispiro-1,2,4-trioxolanes. <i>Journal of Molecular Graphics and Modelling</i> , 2008, 27, 394-400. | 1.3 | 11 |
| 3449 | From lithium ketazides to isomeric silylketazine-rings – imine-enamine tautomerism. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 197-204. | 0.8 | 2 |
| 3450 | The influence of the ligand structure on activation of hafnocene polymerization catalysts: A theoretical study. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 155-163. | 0.8 | 12 |
| 3451 | Ethylene addition to group-6 transition metal oxo complexes – A theoretical study. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 737-749. | 0.8 | 16 |
| 3452 | The differences in solid state structures of C,N-chelated nbutyltin(IV) fluorides. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 2937-2941. | 0.8 | 13 |
| 3453 | Quantum chemical study of ethylene addition to group-7 oxo complexes MO ₂ (CH ₃)(CH ₂) (M=Mn, Tc). <i>Journal of Organometallic Chemistry</i> , 2008, 693, 3697-3702. | 0.8 | 13 |
| 3454 | On the role of the indenyl effect in controlling intramolecular hydride transfer in iron carbonyl complexes. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 3697-3702. | 0.8 | 5 |
| 3455 | Influence of the ligand structure of hafnocene polymerization catalysts: A theoretical study on chain termination reactions in ethene polymerization. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 3915-3922. | 0.8 | 11 |
| 3456 | Theoretical investigation of the photosensitization mechanisms of urocanic acid. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2008, 91, 96-98. | 1.7 | 11 |
| 3457 | The photophysics of flavins: What makes the difference between gas phase and aqueous solution?. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2008, 198, 221-231. | 2.0 | 93 |
| 3458 | Density functional theory on the larger active site models for [NiFe] hydrogenases: Two-state reactivity?. <i>Comptes Rendus Chimie</i> , 2008, 11, 790-804. | 0.2 | 39 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3459 | An ab initio study of the interaction of DNA fragments with methyllithium. <i>Comptes Rendus Chimie</i> , 2008, 11, 1262-1270. | 0.2 | 2 |
| 3460 | Theoretical exploration of the photosensitive properties of xanthurenic acid, a tryptophan metabolite in cataractous human lenses. <i>Dyes and Pigments</i> , 2008, 76, 646-649. | 2.0 | 13 |
| 3461 | Induced solvent chirality: A VCD study of camphor in CDCl ₃ . <i>Chemical Physics Letters</i> , 2008, 450, 426-430. | 1.2 | 60 |
| 3462 | Microsolvation of the Zn(II) ion in aqueous solution: A hybrid QM/MM MD approach using non-periodic boundary conditions. <i>Chemical Physics Letters</i> , 2008, 451, 53-57. | 1.2 | 20 |
| 3463 | A first principle study of terahertz (THz) spectra of acephate. <i>Chemical Physics Letters</i> , 2008, 452, 59-66. | 1.2 | 34 |
| 3464 | Solvent effects on zero-point vibrational corrections to optical rotations and nuclear magnetic resonance shielding constants. <i>Chemical Physics Letters</i> , 2008, 451, 226-232. | 1.2 | 50 |
| 3465 | Structural and vibrational determination of small gallium-arsenide clusters from CCSD(T) and DFT calculations. <i>Chemical Physics Letters</i> , 2008, 453, 49-54. | 1.2 | 17 |
| 3466 | A discrete/continuum QM/MM MD study of the triplet state of acetone in aqueous solution. <i>Chemical Physics Letters</i> , 2008, 453, 202-206. | 1.2 | 12 |
| 3467 | Analytical representation of the Becke-Roussel exchange functional. <i>Chemical Physics Letters</i> , 2008, 455, 103-109. | 1.2 | 25 |
| 3468 | The recognition of a new pathway for the reaction of molecular oxygen with a Pd(II)-hydride to produce a Pd(II)-hydroperoxide. <i>Chemical Physics Letters</i> , 2008, 456, 41-46. | 1.2 | 15 |
| 3469 | Modelling organic molecular crystals by hybrid quantum mechanical/molecular mechanical embedding. <i>Chemical Physics Letters</i> , 2008, 457, 154-158. | 1.2 | 15 |
| 3470 | DFT study of the spin-forbidden reaction of N ₂ O and CO catalyzed by Pt ⁺ . <i>Chemical Physics Letters</i> , 2008, 460, 13-17. | 1.2 | 17 |
| 3471 | Spin-orbit coupling in keto-porphyrins. <i>Chemical Physics Letters</i> , 2008, 458, 190-194. | 1.2 | 7 |
| 3472 | Gas-phase ion chemistry of BF ₃ /CH ₄ mixtures: Activation of methane by $\langle \text{mml:math altimg="si1.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/cg" \rangle$ | 1.2 | 7 |
| 3473 | Spectroscopy and dissociation of HX ₂ ⁺ (X = Cl, Br, I). <i>Chemical Physics Letters</i> , 2008, 461, 348-352. | 1.2 | 6 |
| 3474 | Clusters of hafnium, Hf _n = 2-8. <i>Chemical Physics Letters</i> , 2008, 462, 183-187. | 1.2 | 9 |
| 3475 | Range-separation by the Yukawa potential in long-range corrected density functional theory with Gaussian-type basis functions. <i>Chemical Physics Letters</i> , 2008, 462, 348-351. | 1.2 | 67 |
| 3476 | Theoretical analysis of the solid-state terahertz spectrum of the high explosive RDX. <i>Chemical Physics Letters</i> , 2008, 463, 84-89. | 1.2 | 60 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3477 | Mechanisms for the Ni ⁺ -mediated oxidation of benzene to phenol by N ₂ O. <i>Chemical Physics Letters</i> , 2008, 463, 54-59. | 1.2 | 5 |
| 3478 | Effects of protonation and deprotonation on the excitation energies of lumiflavin. <i>Chemical Physics Letters</i> , 2008, 463, 400-404. | 1.2 | 28 |
| 3479 | The gas-phase catalytic formation of H ₂ by cations. <i>Chemical Physics Letters</i> , 2008, 463, 327-329. | 1.2 | 1 |
| 3480 | Terahertz spectroscopy and molecular modeling of 2-pyridone clusters. <i>Chemical Physics Letters</i> , 2008, 464, 171-176. | 1.2 | 8 |
| 3481 | Quantum Monte Carlo study of the cooperative binding of NO ₂ to fragment models of carbon nanotubes. <i>Chemical Physics Letters</i> , 2008, 466, 170-175. | 1.2 | 9 |
| 3482 | Structures and electron detachment energies of Ga ₂ S ₃ ⁻ and Ga ₃ S ₂ ⁻ . <i>Chemical Physics Letters</i> , 2008, 467, 23-27. | 1.2 | 9 |
| 3483 | Synthesis, biological evaluation and molecular modelling studies of methyleneimidazole substituted biaryls as inhibitors of human 17 β -hydroxylase-17,20-lyase (CYP17). Part I: Heterocyclic modifications of the core structure. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 1992-2010. | 1.4 | 76 |
| 3484 | Synthesis, biological evaluation, and molecular modeling studies of methylene imidazole substituted biaryls as inhibitors of human 17 β -hydroxylase-17,20-lyase (CYP17) Part II: Core rigidification and influence of substituents at the methylene bridge. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 7715-7727. | 1.4 | 58 |
| 3485 | Multivariate characterisation and quantitative structure-property relationship modelling of nitroaromatic compounds. <i>Analytica Chimica Acta</i> , 2008, 621, 155-162. | 2.6 | 6 |
| 3486 | A comparative study of single reference correlation methods of the coupled-pair type. <i>Chemical Physics</i> , 2008, 343, 217-230. | 0.9 | 96 |
| 3487 | Hydrogen and dihydrogen bonding of transition metal hydrides. <i>Chemical Physics</i> , 2008, 345, 95-102. | 0.9 | 30 |
| 3488 | Deactivation via ring opening: A quantum chemical study of the excited states of furan and comparison to thiophene. <i>Chemical Physics</i> , 2008, 349, 269-277. | 0.9 | 58 |
| 3489 | A density functional investigation of the structural and vibrational properties of the highly symmetric molecules M ₄ O ₆ , M ₄ O ₁₀ (M=P, As, Sb, Bi). <i>Vibrational Spectroscopy</i> , 2008, 48, 135-141. | 1.2 | 5 |
| 3490 | FRET-derived ratiometric fluorescence sensor for Cu ²⁺ . <i>Tetrahedron</i> , 2008, 64, 1294-1300. | 1.0 | 121 |
| 3491 | The influence of exocyclic phosphorous substituents on the intrinsic stability of four-membered heterophosphetes: a theoretical study. <i>Tetrahedron</i> , 2008, 64, 1868-1878. | 1.0 | 11 |
| 3492 | Umpolung catalysis: assessment of catalyst and substrate reactivities in acyloin type reactions. <i>Tetrahedron</i> , 2008, 64, 1648-1653. | 1.0 | 19 |
| 3493 | Bidentate phosphines as ligands in the palladium-catalyzed intramolecular arylation: the intermolecular base-assisted proton abstraction mechanism. <i>Tetrahedron</i> , 2008, 64, 6021-6029. | 1.0 | 123 |
| 3494 | A computational study of lithium methoxide mixed aggregates with alkyllithiums. <i>Tetrahedron</i> , 2008, 64, 5314-5321. | 1.0 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3495 | Sigmatropic shifts and cycloadditions on neutral, cationic, and anionic pentadienyl+butadiene potential energy surfaces. <i>Tetrahedron</i> , 2008, 64, 5672-5679. | 1.0 | 16 |
| 3496 | Theory-guided design of Brønsted acid-assisted phosphine catalysis: synthesis of dihydropyrones from aldehydes and allenolates. <i>Tetrahedron</i> , 2008, 64, 6935-6942. | 1.0 | 50 |
| 3497 | Mechanistic insights into the transmetalation step of a Suzuki–Miyaura reaction of 2(4)-bromopyridines: characterization of an intermediate. <i>Tetrahedron</i> , 2008, 64, 7437-7443. | 1.0 | 66 |
| 3498 | Donor–acceptor benzothiazole-derived dyes with an extended heteroaryl-containing conjugated system: synthesis, DFT study and antimicrobial activity. <i>Tetrahedron</i> , 2008, 64, 10605-10618. | 1.0 | 71 |
| 3499 | Thermal isomerization of dewarbenzene derivatives. <i>Tetrahedron Letters</i> , 2008, 49, 4130-4133. | 0.7 | 10 |
| 3500 | The prediction of gas-phase and aqueous basicities for alkyl amines. <i>Computational and Theoretical Chemistry</i> , 2008, 849, 84-97. | 1.5 | 9 |
| 3501 | Explaining the HOMO and LUMO distribution on individual ligands in mer-Alq ₃ and its α -CH ₃ -N substituted derivatives. <i>Computational and Theoretical Chemistry</i> , 2008, 850, 79-83. | 1.5 | 16 |
| 3502 | Origin of reverse stability of diphosphouracil tautomers compared to their analogue uracil: DFT and ab initio study. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 54-62. | 1.5 | 9 |
| 3503 | Photophysical and photochemical properties of anthraquinones: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 220-224. | 1.5 | 12 |
| 3504 | Theoretical exploration on quenching mechanisms of triplet state riboflavin by xanthone derivatives. <i>Computational and Theoretical Chemistry</i> , 2008, 854, 106-109. | 1.5 | 2 |
| 3505 | DFT analysis of rotational barriers, ¹ H and ¹³ C NMR chemical shifts in neutral and protonated furfurylidenanilines. <i>Computational and Theoretical Chemistry</i> , 2008, 852, 78-82. | 1.5 | 3 |
| 3506 | On the calculation of ¹⁵ N chemical shifts using linear regression formulae. A performance comparison of different methods. <i>Computational and Theoretical Chemistry</i> , 2008, 856, 1-8. | 1.5 | 7 |
| 3507 | Assessment of density functionals, semiempirical methods, and SCC-DFTB for protonated creatinine geometries. <i>Computational and Theoretical Chemistry</i> , 2008, 861, 68-73. | 1.5 | 11 |
| 3508 | Thermodynamic investigation of the gas-phase reactions in the chemical vapor deposition of boron carbide with BCl ₃ -CH ₄ -H ₂ precursors. <i>Computational and Theoretical Chemistry</i> , 2008, 861, 103-116. | 1.5 | 25 |
| 3509 | Theoretical investigation on the triplet excited state properties of the porphyrin-related photosensitizers and the implications in illustrating their photosensitization mechanisms. <i>Computational and Theoretical Chemistry</i> , 2008, 862, 130-132. | 1.5 | 10 |
| 3510 | A comparative post-Hartree–Fock and density functional theory study of monochalcogenide diatomic molecules. <i>Computational and Theoretical Chemistry</i> , 2008, 863, 79-83. | 1.5 | 7 |
| 3511 | The theoretical investigation on gas-phase chemistry of YNH ⁺ with propene. <i>Computational and Theoretical Chemistry</i> , 2008, 866, 5-10. | 1.5 | 3 |
| 3512 | DFT study of NLO properties of boroxine based octupolar molecules. <i>Computational and Theoretical Chemistry</i> , 2008, 866, 58-62. | 1.5 | 15 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3513 | Some electronic properties of saturated and unsaturated cubane oligomers using DFT-based calculations. <i>Computational and Theoretical Chemistry</i> , 2008, 868, 37-41. | 1.5 | 9 |
| 3514 | Theoretical investigation for the reaction of NO ₂ (2A ₁) with CO(1 \hat{a} +) catalyzed by Ti+(X ₄ F). <i>Computational and Theoretical Chemistry</i> , 2008, 869, 89-93. | 1.5 | 10 |
| 3515 | Hybrid-DFT study for the initial oxidation steps on silicon cluster surface. <i>Applied Surface Science</i> , 2008, 254, 7909-7912. | 3.1 | 0 |
| 3516 | Influence of the microstructure of several substrates on the SERS effect of p-hydroxybenzoic acid adsorbed on Ag nanoparticles. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2008, 316, 253-257. | 2.3 | 5 |
| 3517 | Quantitative structure-property relationships for the reactivity parameters of acrylate monomers. <i>European Polymer Journal</i> , 2008, 44, 3997-4001. | 2.6 | 27 |
| 3518 | The electronic structure of Ti(BH ₄) ₃ : Photoelectron spectra and calculation of vertical ionization energies. <i>Inorganica Chimica Acta</i> , 2008, 361, 462-466. | 1.2 | 7 |
| 3519 | Norbornadiene complexes of molybdenum(II) and their transformation to a catalyst for ring-opening metathesis polymerization: DFT calculations and X-ray crystal structure of a new norbornadiene complex [MoCl(GeCl ₃)(CO) ₃ (<i>i</i> -4-nbd)]. <i>Inorganica Chimica Acta</i> , 2008, 361, 502-512. | 1.2 | 20 |
| 3520 | On the oxidation of alkyl and aryl sulfides by [(Me ₃ TACN)MnVO(OH) ₂] ⁺ : A density functional study. <i>Inorganica Chimica Acta</i> , 2008, 361, 1079-1086. | 1.2 | 11 |
| 3521 | Experimental and computational studies of two new mono- and dinuclear iridium complexes containing a Buchwald biphenyl phosphine ligand. <i>Inorganica Chimica Acta</i> , 2008, 361, 2623-2630. | 1.2 | 5 |
| 3522 | Electron capture, femtosecond electron transfer and theory: A study of noncovalent crown ether 1, <i>n</i> -diammonium alkane complexes. <i>International Journal of Mass Spectrometry</i> , 2008, 276, 116-126. | 0.7 | 32 |
| 3523 | Paired interacting orbitals (PIO) study of molybdena-alumina system active in alkene metathesis. <i>Journal of Molecular Catalysis A</i> , 2008, 284, 8-15. | 4.8 | 8 |
| 3524 | Spectroscopic properties of N-n-hexyltetrachlorophthalimide and supramolecular interactions in its crystals. <i>Journal of Molecular Structure</i> , 2008, 874, 145-150. | 1.8 | 5 |
| 3525 | Prototropic equilibrium between 1-H-2-oxo-pyrido[2,1-b][3,4]dihydropyrimidinium chloride and 3-(2-aminopyridinium)propionate hydrochloride studied by X-ray, FTIR, Raman, NMR and ab initio methods. <i>Journal of Molecular Structure</i> , 2008, 875, 244-253. | 1.8 | 5 |
| 3526 | Experimental and theoretical determination of the antioxidant properties of isoespintanol (2-isopropyl-3,6-dimethoxy-5-methylphenol). <i>Journal of Molecular Structure</i> , 2008, 877, 1-6. | 1.8 | 51 |
| 3527 | Spectroscopic characterization and single molecule structures of N,N-bis-(3-phthalimidopropyl)-N-(2-hydroxyethyl)-N-propylammonium salts and their hydrates. <i>Journal of Molecular Structure</i> , 2008, 879, 7-13. | 1.8 | 1 |
| 3528 | Experimental and ab-initio studies of the spectroscopic properties of N,N,N ⁺ -triphenylguanidine and N,N,N ⁺ -triphenylguanidinium chloride. <i>Journal of Molecular Structure</i> , 2008, 878, 169-176. | 1.8 | 12 |
| 3529 | Crystal and molecular structure, hydrogen bond and electrostatic interactions of bis(1-methylisonicotinate)hydrogen perchlorate studied by X-ray diffraction, DFT calculations, FT-IR, Raman and NMR spectroscopies. <i>Journal of Molecular Structure</i> , 2008, 880, 77-85. | 1.8 | 18 |
| 3530 | DFT, FTIR, Raman and NMR study of 1-methyl-8-oxyquinolinium betaine. <i>Journal of Molecular Structure</i> , 2008, 887, 20-33. | 1.8 | 7 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 3531 | Molecular structure, hydrogen bonding and spectroscopic properties of the complex of piperidine-4-carboxylic acid with chloroacetic acid. <i>Journal of Molecular Structure</i> , 2008, 889, 112-118. | 1.8 | 9 |
| 3532 | The structure of betaxolol from single crystal X-ray diffraction and natural bond orbital analysis. <i>Journal of Molecular Structure</i> , 2008, 891, 437-442. | 1.8 | 10 |
| 3533 | DFT and time-resolved IR investigation of electron transfer between photogenerated 17- and 19-electron organometallic radicals. <i>Journal of Molecular Structure</i> , 2008, 890, 328-338. | 1.8 | 10 |
| 3534 | Density Functionals with Broad Applicability in Chemistry. <i>Accounts of Chemical Research</i> , 2008, 41, 157-167. | 7.6 | 6,193 |
| 3535 | Microsolvation of Glycine: A DFT Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3722-3730. | 1.1 | 130 |
| 3536 | Crown Ether Inclusion Complexes of the Early Actinide Elements, [AnO ₂ (18-crown-6)] ⁿ⁺ , An = U, Np, Pu and <i>n</i> = 1, 2: A Relativistic Density Functional Study. <i>Inorganic Chemistry</i> , 2008, 47, 1465-1475. | 1.9 | 117 |
| 3537 | Orbital-dependent density functionals: Theory and applications. <i>Reviews of Modern Physics</i> , 2008, 80, 3-60. | 16.4 | 1,069 |
| 3538 | TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes: Conventional versus Long-Range Hybrids. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 123-135. | 2.3 | 766 |
| 3539 | Configurational Labile Lithiated <i>O</i> -Benzyl Carbamates: Application in Asymmetric Synthesis and Quantum Chemical Investigations on the Equilibrium of Diastereomers. <i>Chemistry - an Asian Journal</i> , 2008, 3, 78-87. | 1.7 | 30 |
| 3540 | DFT Studies on the Borylation of α,β -Unsaturated Carbonyl Compounds Catalyzed by Phosphine Copper(I) Boryl Complexes and Observations on the Interconversions between O- and C-Bound Enolates of Cu, B, and Si. <i>Organometallics</i> , 2008, 27, 4443-4454. | 1.1 | 210 |
| 3541 | Excited states of thiophene: ring opening as deactivation mechanism. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 380-392. | 1.3 | 86 |
| 3542 | Mechanism of Air Oxidation of the Fragrance Terpene Geraniol. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 101-106. | 2.3 | 34 |
| 3543 | 9,10-Dihydroplatinanthracenes with Aromatic Diimine Ligands: Syntheses and Spectroscopic and Computational Studies of New Luminescent Materials. <i>Organometallics</i> , 2008, 27, 1765-1779. | 1.1 | 22 |
| 3544 | Excitation energies in density functional theory: An evaluation and a diagnostic test. <i>Journal of Chemical Physics</i> , 2008, 128, 044118. | 1.2 | 1,190 |
| 3545 | Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 6615. | 1.3 | 10,464 |
| 3546 | Synthesis of Tricyclic Phosphonopyrrolidines via IMDAF: Experimental and Theoretical Investigation of the Observed Stereoselectivity. <i>Journal of Organic Chemistry</i> , 2008, 73, 7921-7927. | 1.7 | 12 |
| 3547 | Performance of B3LYP Density Functional Methods for a Large Set of Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 297-306. | 2.3 | 931 |
| 3548 | Comparison of Time-Dependent Density-Functional Theory and Coupled Cluster Theory for the Calculation of the Optical Rotations of Chiral Molecules. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1339-1345. | 1.1 | 98 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3549 | Secondary Bonding Interactions in Biomimetic [2Fe ²⁺ 2S] Clusters. <i>Inorganic Chemistry</i> , 2008, 47, 1586-1596. | 1.9 | 24 |
| 3550 | Synthesis, structure, and properties of new phosphorus Schiff bases. <i>Russian Journal of General Chemistry</i> , 2008, 78, 567-574. | 0.3 | 3 |
| 3551 | Mechanistic possibilities for oxetane formation in the biosynthesis of Taxol's D ring. <i>Russian Journal of General Chemistry</i> , 2008, 78, 723-731. | 0.3 | 15 |
| 3552 | Synthesis, structure, and complexing ability of pyrrole-2-carbaldehyde ferrocenoylhydrazone. <i>Russian Journal of General Chemistry</i> , 2008, 78, 1586-1593. | 0.3 | 8 |
| 3553 | Molecular and crystal structure of 1-amino-X-pyrazinium mesitylenesulfonates. <i>Russian Journal of Organic Chemistry</i> , 2008, 44, 292-301. | 0.3 | 8 |
| 3554 | The thermodynamic stability of the LaBr ₄ ⁻ ion. <i>Russian Journal of Physical Chemistry A</i> , 2008, 82, 767-772. | 0.1 | 7 |
| 3555 | Quantum-chemical calculations of the structure of trioxyl radicals. <i>Russian Journal of Physical Chemistry A</i> , 2008, 82, 1277-1282. | 0.1 | 8 |
| 3556 | Estimation of reliability of quantum-chemical calculations of electronic transitions in aqua complexes of transition metals. <i>Russian Journal of Electrochemistry</i> , 2008, 44, 1105-1112. | 0.3 | 12 |
| 3557 | A Molecular Basis for Agonist and Antagonist Actions at GABA _C Receptors. <i>Chemical Biology and Drug Design</i> , 2008, 71, 306-327. | 1.5 | 46 |
| 3558 | Synthesis, characterization, and studies on DNA binding of a new Mg(II) complex with N1,N8-bis(1-methyl-4-nitropyrrole-2-carbonyl)triethylenetetramine. <i>Biochemistry (Moscow)</i> , 2008, 73, 245-251. | 0.7 | 2 |
| 3559 | Molecular Dynamic Investigation of the Interaction of Supported Affinity Ligands with Monoclonal Antibodies. <i>Biotechnology Progress</i> , 2008, 24, 527-539. | 1.3 | 29 |
| 3560 | Mechanistic analogies and differences between gold- and palladium-supported Schiff base complexes as hydrogenation catalysts: A combined kinetic and DFT study. <i>Journal of Catalysis</i> , 2008, 254, 226-237. | 3.1 | 29 |
| 3561 | DFT at Its Best: Metal- versus Ligand-Centered Reduction in Nickel Hydroporphyrins. <i>Journal of Physical Chemistry B</i> , 2008, 112, 15158-15173. | 1.2 | 20 |
| 3562 | Highly Accurate First-Principles Benchmark Data Sets for the Parametrization and Validation of Density Functional and Other Approximate Methods. Derivation of a Robust, Generally Applicable, Double-Hybrid Functional for Thermochemistry and Thermochemical Kinetics. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12868-12886. | 1.1 | 680 |
| 3563 | Mechanism of Molecular Oxygen Reduction at the Cathode of a PEM Fuel Cell: Non-Electrochemical Reactions on Catalytic Pt Particles. <i>Journal of Physical Chemistry C</i> , 2008, 112, 8464-8475. | 1.5 | 48 |
| 3564 | DFT Approach to the Calculation of Mössbauer Isomer Shifts. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 278-285. | 2.3 | 40 |
| 3565 | Computational Analysis of Amine-Borane Adducts as Potential Hydrogen Storage Materials with Reversible Hydrogen Uptake. <i>Inorganic Chemistry</i> , 2008, 47, 5910-5918. | 1.9 | 91 |
| 3566 | 2-(4,5,6,7-Tetrafluorobenzimidazol-2-yl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazole-3-oxide-1-oxyl, A Hydrogen-Bonded Organic Quasi-1D Ferromagnet. <i>Journal of the American Chemical Society</i> , 2008, 130, 186-194. | 6.6 | 34 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3567 | A DFT Perspective on the Structures and Electronic Spectra of the Orange and Blue Isomers of Photochromic Dithizonatophenylmercury(II). <i>Journal of Physical Chemistry A</i> , 2008, 112, 2211-2218. | 1.1 | 22 |
| 3568 | Orbital Views of the Electron Transport in Molecular Devices. <i>Journal of the American Chemical Society</i> , 2008, 130, 9406-9413. | 6.6 | 223 |
| 3569 | Activation of CS ₂ and CS by ML ₃ Complexes. <i>Journal of the American Chemical Society</i> , 2008, 130, 11928-11938. | 6.6 | 37 |
| 3570 | Triplet and ground state potential energy surfaces of 1,4-diphenyl-1,3-butadiene: theory and experiment. <i>Photochemical and Photobiological Sciences</i> , 2008, 7, 566-577. | 1.6 | 14 |
| 3571 | Defining the Electronic and Geometric Structure of One-Electron Oxidized Copper ^{II} -Bis-phenoxide Complexes. <i>Journal of the American Chemical Society</i> , 2008, 130, 15448-15459. | 6.6 | 162 |
| 3572 | Theoretical and Experimental Studies on the Mechanism of Norbornadiene Pauson ^{III} -Khand Cycloadducts Photorearrangement. Is There a Pathway on the Excited Singlet Potential Energy Surface?. <i>Journal of the American Chemical Society</i> , 2008, 130, 16898-16907. | 6.6 | 5 |
| 3573 | In Search of Efficient 5-Endo-dig Cyclization of a Carbon-Centered Radical: 40 Years from a Prediction to Another Success for the Baldwin Rules. <i>Journal of the American Chemical Society</i> , 2008, 130, 10984-10995. | 6.6 | 67 |
| 3574 | Novel Iron(III) Porphyrazine Complex. Complex Speciation and Reactions with NO and H ₂ O ₂ . <i>Inorganic Chemistry</i> , 2008, 47, 2994-3013. | 1.9 | 61 |
| 3575 | Structural and Electronic Characteristics of Perhydrogenated Boron Nitride Nanotubes. <i>Journal of Physical Chemistry C</i> , 2008, 112, 2418-2422. | 1.5 | 17 |
| 3576 | Real-Time Propagation of the Reduced One-Electron Density Matrix in Atom-Centered Orbitals: Application to Multielectron Dynamics of Carbon Clusters C _n in the Strong Laser Pulses. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10442-10447. | 1.1 | 9 |
| 3577 | Electrochemical Oxidation of 2-Pyrimidinethiols and Theoretical Study of Their Dimers, Disulfides, Sulfenyl Radicals, and Tautomers. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1643-1655. | 1.1 | 11 |
| 3578 | Polyiodides and Polytellurides: Analogies and Differences. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2008, 183, 1036-1045. | 0.8 | 5 |
| 3579 | Nanojets, Electrospray, and Ion Field Evaporation: Molecular Dynamics Simulations and Laboratory Experiments. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9628-9649. | 1.1 | 91 |
| 3580 | Generalized gradient approximation model exchange holes for range-separated hybrids. <i>Journal of Chemical Physics</i> , 2008, 128, 194105. | 1.2 | 238 |
| 3581 | A New Cyclization to Fused Pyrazoles Tunable for Pericyclic or Pseudopericyclic Route: An Experimental and Theoretical Study. <i>Journal of Organic Chemistry</i> , 2008, 73, 3900-3906. | 1.7 | 13 |
| 3582 | The Curtius Rearrangement of Cyclopropyl and Cyclopropenoyl Azides. A Combined Theoretical and Experimental Mechanistic Study. <i>Journal of Organic Chemistry</i> , 2008, 73, 8189-8197. | 1.7 | 31 |
| 3583 | Quantum Monte Carlo study of porphyrin transition metal complexes. <i>Journal of Chemical Physics</i> , 2008, 129, 085103. | 1.2 | 19 |
| 3584 | Unusual Selectivity-Determining Factors in the Phosphine-Free Heck Arylation of Allyl Ethers. <i>Organometallics</i> , 2008, 27, 3187-3195. | 1.1 | 28 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3585 | DFT Calculation of ^{119}Sn , ^{13}C and ^2J (^{119}Sn , ^1H) Coupling Constants in Di- and Trimethyltin(IV) Compounds. <i>Inorganic Chemistry</i> , 2008, 47, 4796-4807. | 1.9 | 46 |
| 3586 | Quantum Chemical Approach to the Mechanism for the Biological Conversion of Tyrosine to Dopaquinone. <i>Journal of the American Chemical Society</i> , 2008, 130, 16890-16897. | 6.6 | 70 |
| 3587 | Performance of the Density Functional Theory/Multireference Configuration Interaction Method on Electronic Excitation of Extended π -Systems. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1501-1515. | 2.3 | 164 |
| 3588 | Reaction Electronic Flux: A New Concept To Get Insights into Reaction Mechanisms. Study of Model Symmetric Nucleophilic Substitutions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11801-11807. | 1.1 | 100 |
| 3589 | The Coupling of Isonitriles and Carboxylic Acids Occurring By Sequential Concerted Rearrangement Mechanisms. <i>Organic Letters</i> , 2008, 10, 4093-4096. | 2.4 | 62 |
| 3590 | Consequences of Spin Contamination in Unrestricted Calculations on Open-Shell Species: Effect of Hartree-Fock and Møller-Plesset Contributions in Hybrid and Double-Hybrid Density Functional Theory Approaches. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13225-13230. | 1.1 | 137 |
| 3591 | Basis Set Convergence of Nuclear Magnetic Shielding Constants Calculated by Density Functional Methods. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 719-727. | 2.3 | 320 |
| 3592 | Performance of SM8 on a Test To Predict Small-Molecule Solvation Free Energies. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8651-8655. | 1.2 | 56 |
| 3593 | Sigma Stellation: A Design Strategy for Electron Boxes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 983-988. | 1.1 | 29 |
| 3594 | Electrostatic control of proton pumping in cytochrome c oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2008, 1777, 277-284. | 0.5 | 47 |
| 3595 | Reactivity of $(\text{TiO})_2\text{N}$ Clusters ($n = 1-10$): Probing Gas-Phase Acidity and Basicity Properties. <i>Journal of Physical Chemistry C</i> , 2008, 112, 16087-16095. | 1.5 | 66 |
| 3596 | $\text{Ca}^{2+}\text{Na}^+\text{Cu}^{2+}$ | 1.1 | 17 |
| 3597 | Combined Ligand Field and Density Functional Theory Analysis of the Magnetic Anisotropy in Oligonuclear Complexes Based on $\text{Fe}^{\text{III}}\text{CN}^{\text{I}}\text{M}^{\text{II}}$ Exchange-Coupled Pairs. <i>Inorganic Chemistry</i> , 2008, 47, 2449-2463. | 1.9 | 78 |
| 3598 | Ground state of octahedral platinum hexafluoride. <i>Physical Review A</i> , 2008, 77, . | 1.0 | 38 |
| 3599 | Accurate Benchmark Calculation of the Reaction Barrier Height for Hydrogen Abstraction by the Hydroperoxyl Radical from Methane. Implications for $\text{C}_2\text{H}_2 + \text{HO}_2$ where $n = 2-4$. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7047-7054. | 1.1 | 105 |
| 3600 | Theoretical Study of 5-Aminolevulinic Acid Tautomerization: A Novel Self-Catalyzed Mechanism. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4367-4374. | 1.1 | 2 |
| 3601 | Addition of POSS_8 to the Si(100) Surface. <i>Journal of Physical Chemistry C</i> , 2008, 112, 754-761. | 1.5 | 6 |
| 3602 | Structural Characteristics of Perhydrogenated Boron Nitride Fullerenes. <i>Journal of Physical Chemistry C</i> , 2008, 112, 10032-10037. | 1.5 | 21 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3603 | Substituent Effects on Singlet \rightarrow Triplet Gaps and Mechanisms of 1,2-Rearrangements of 1,3-Oxazol-2-ylidenes to 1,3-Oxazoles. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8775-8784. | 1.1 | 19 |
| 3604 | Analysis of H $\frac{1}{2}$ ckel $\hat{\epsilon}$ ™s [4<i>n</i> + 2] Rule through Electronic Delocalization Measures. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13231-13238. | 1.1 | 38 |
| 3605 | Developing <i>ab initio</i> quality force fields from condensed phase quantum-mechanics/molecular-mechanics calculations through the adaptive force matching method. <i>Journal of Chemical Physics</i> , 2008, 129, 064108. | 1.2 | 106 |
| 3606 | Shedding light on octathio[8]circulene and some of its plate-like derivatives. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 1743. | 1.3 | 43 |
| 3607 | Accurate Spin-State Energies for Iron Complexes. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 2057-2066. | 2.3 | 327 |
| 3608 | OH Formation from O and H Atoms Physisorbed on a Graphitic Surface through the Langmuir \rightarrow Hinshelwood Mechanism: A Quasi-Classical Approach. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11921-11930. | 1.1 | 38 |
| 3609 | On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters. II. The water hexamer and van der Waals interactions. <i>Journal of Chemical Physics</i> , 2008, 129, 194111. | 1.2 | 211 |
| 3610 | The Modeling of Molecules Through Computational Methods. , 2008, , 229-274. | | 0 |
| 3611 | Self-consistent treatment of spin $\hat{\epsilon}$ orbit interactions with efficient Hartree $\hat{\epsilon}$ Fock and density functional methods. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 1748. | 1.3 | 145 |
| 3612 | Magnetic exchange couplings from noncollinear spin density functional perturbation theory. <i>Journal of Chemical Physics</i> , 2008, 129, 194107. | 1.2 | 24 |
| 3613 | Heterocycle-Based Isomeric Chromophores with Substantially Varying NLO Properties: A New Structure \rightarrow Property Correlation Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4844-4852. | 1.1 | 33 |
| 3614 | Role of Negative Hyperconjugation and Anomeric Effects in the Stabilization of the Intermediate in S _N V Reactions. <i>Journal of Organic Chemistry</i> , 2008, 73, 2980-2994. | 1.7 | 21 |
| 3615 | Aggregation Behavior of Octyl Viologen Di[bis(trifluoromethanesulfonyl)amide] in Nonpolar Solvents. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16566-16574. | 1.2 | 21 |
| 3616 | Synthesis, Crystal Structure, EPR and DFT Studies, and Redox Properties of [2]Tetramethylsilacobaltocenophane. <i>Organometallics</i> , 2008, 27, 6427-6433. | 1.1 | 31 |
| 3617 | Laser-induced nuclear magnetic resonance splitting in hydrocarbons. <i>Journal of Chemical Physics</i> , 2008, 129, 124102. | 1.2 | 26 |
| 3618 | Orbital energies and negative electron affinities from density functional theory: Insight from the integer discontinuity. <i>Journal of Chemical Physics</i> , 2008, 129, 044110. | 1.2 | 112 |
| 3619 | Preparation of tris(azolyl)phosphine gold(<sc>i</sc>) complexes: digold(<sc>i</sc>) coordination and variation in solid state intermolecular interactions. <i>New Journal of Chemistry</i> , 2008, 32, 138-150. | 1.4 | 13 |
| 3620 | Azo \rightarrow Hydrazone Tautomerism in Protonated Aminoazobenzenes: Resonance Raman Spectroscopy and Quantum-Chemical Calculations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4437-4443. | 1.1 | 69 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3621 | Structural Characterization, Solution Studies, and DFT Calculations on a Series of Binuclear Gold(III) Oxo Complexes: Relationships to Biological Properties. <i>Inorganic Chemistry</i> , 2008, 47, 2368-2379. | 1.9 | 102 |
| 3622 | Theoretical Study of the Oxygen Exchange in Uranyl Hydroxide. An Old Riddle Solved?. <i>Journal of the American Chemical Society</i> , 2008, 130, 13735-13744. | 6.6 | 61 |
| 3623 | Computational Studies on Biosynthetic Carbocation Rearrangements Leading to Sativene, Cyclosativene, Î±-Ylangene, and Î²-Ylangene. <i>Journal of Organic Chemistry</i> , 2008, 73, 6570-6579. http://www.w3.org/1998/Math/MathML | 1.7 | 57 |
| 3624 | SrTiO_3 BaTiO_3 using the projector augmented wave method: Performance of hybrid and semilocal functionals. <i>Physical Review B</i> , 2008, 78, . | 1.1 | 25 |
| 3625 | Complete Mechanism of Î¶* Intramolecular Aromatic Hydroxylation through O ₂ Activation by a Macrocyclic Dicopper(I) Complex. <i>Journal of the American Chemical Society</i> , 2008, 130, 17710-17717. | 6.6 | 62 |
| 3626 | DFT-UX3LYP Studies on the Coordination Chemistry of Ni ²⁺ . Part 1: Six Coordinate [Ni(NH ₃) ₃] _n (H ₂ O) _{6-n} ²⁺ Complexes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10657-10666. | 1.1 | 61 |
| 3627 | Exploring the Limit of Accuracy of the Global Hybrid Meta Density Functional for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1849-1868. | 2.3 | 956 |
| 3628 | Effect of Spin-Orbit Coupling on Reduction Potentials of Octahedral Ruthenium(II/III) and Osmium(II/III) Complexes. <i>Journal of the American Chemical Society</i> , 2008, 130, 10947-10954. | 6.6 | 50 |
| 3630 | The cobalt-doped aluminum Al _n Co (n=8-16) and their anions: Structure, thermochemistry, and electron affinities. <i>Journal of Alloys and Compounds</i> , 2008, 466, 463-470. | 2.8 | 9 |
| 3631 | Pd(I) Phosphine Carbonyl and Hydride Complexes Implicated in the Palladium-Catalyzed Oxo Process. <i>Journal of the American Chemical Society</i> , 2008, 130, 10612-10624. | 6.6 | 41 |
| 3632 | The Reaction Mechanism of the Hydroamination of Alkenes Catalyzed by Gold(I)-Phosphine: The Role of the Counterion and the N-Nucleophile Substituents in the Proton-Transfer Step. <i>Journal of the American Chemical Society</i> , 2008, 130, 853-864. | 6.6 | 197 |
| 3633 | Local correlation functional for electrons in two dimensions. <i>Physical Review B</i> , 2008, 78, . | 1.1 | 25 |
| 3634 | Interaction of Coinage Metal Clusters with Chalcogen Dihydrides. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7969-7975. | 1.1 | 37 |
| 3635 | Organocatalytic Enantioselective Diels-Alder Reaction of Dienes with Î±-Diacylamino)acroleins. <i>Organic Letters</i> , 2008, 10, 2893-2896. | 2.4 | 61 |
| 3636 | Electronic structure of copper phthalocyanine: A comparative density functional theory study. <i>Journal of Chemical Physics</i> , 2008, 128, 164107. | 1.2 | 153 |
| 3637 | Importance of the Basis Set for the Spin-State Energetics of Iron Complexes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6384-6391. | 1.1 | 131 |
| 3638 | Synthesis, Reactivity, and Electronic Structure of [Vanadoarenophanes: An Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2008, 130, 11376-11393. | 6.6 | 52 |
| 3639 | Triazolotriazines: a core for luminescent discotic liquid crystals. <i>Chemical Communications</i> , 2008, , 5134. | 2.2 | 71 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3640 | The iron-isotope fractionation dictated by the carboxylic functional: An ab-initio investigation. <i>Geochimica Et Cosmochimica Acta</i> , 2008, 72, 5920-5934. | 1.6 | 19 |
| 3641 | Stereoelectronic Effects on Molecular Geometries and State-Energy Splittings of Ligated Monocopper Dioxygen Complexes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3754-3767. | 1.1 | 58 |
| 3642 | Synthesis of 3,4-benzo-7-hydroxy-2,9-diazabicyclo[3.3.1]non-7-enes by cyclization of 1,3-bis(silyl enol) Tj ETQq0 0 0 rgBT /Overlock 10 T | 1.5 | 9 |
| 3643 | Development and Validation of the B3LYP/N07D Computational Model for Structural Parameter and Magnetic Tensors of Large Free Radicals. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 751-764. | 2.3 | 231 |
| 3644 | An Efficient Methyltrioxorhenium(VII)-Catalyzed Transformation of Hydrotrioxides (ROOOH) into Dihydrogen Trioxide (HOOOH). <i>Journal of the American Chemical Society</i> , 2008, 130, 14086-14087. | 6.6 | 21 |
| 3645 | Hydration Properties of Aqueous Pb(II) Ion. <i>Inorganic Chemistry</i> , 2008, 47, 8233-8241. | 1.9 | 65 |
| 3646 | Zn Coordination Chemistry: Development of Benchmark Suites for Geometries, Dipole Moments, and Bond Dissociation Energies and Their Use To Test and Validate Density Functionals and Molecular Orbital Theory. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 75-85. | 2.3 | 162 |
| 3647 | Assessment of correction methods for the band-gap problem and for finite-size effects in supercell defect calculations: Case studies for ZnO and GaAs. <i>Physical Review B</i> , 2008, 78, . | 1.1 | 1,035 |
| 3648 | Application of the Electrostatically Embedded Many-Body Expansion to Microsolvation of Ammonia in Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 683-688. | 2.3 | 33 |
| 3649 | Systematic optimization of long-range corrected hybrid density functionals. <i>Journal of Chemical Physics</i> , 2008, 128, 084106. | 1.2 | 2,890 |
| 3650 | Assessment of Multicoefficient Correlation Methods, Second-Order Møller-Plesset Perturbation Theory, and Density Functional Theory for H ₃ O ⁺ (H ₂ O) _n (n= 1~5) and OH-(H ₂ O) _n (n= 1~4). <i>Journal of Physical Chemistry B</i> , 2008, 112, 2372-2381. | 1.2 | 29 |
| 3651 | Redefining the atom: atomic charge densities produced by an iterative stockholder approach. <i>Chemical Communications</i> , 2008, , 5909. | 2.2 | 111 |
| 3652 | On the Origin of δ^{\pm} - and δ^2 -Agostic Distortions in Early-Transition-Metal Alkyl Complexes. <i>Organometallics</i> , 2008, 27, 1128-1134. | 1.1 | 54 |
| 3653 | IR/UV spectra and quantum chemical calculations of Trp-Ser: Stacking interactions between backbone and indole side-chain. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2844. | 1.3 | 35 |
| 3654 | Mapping the $d^{\sim}d$ Excited-State Manifolds of Transition Metal δ^2 -Diiminato δ^{\sim} Imido Complexes. Comparison of Density Functional Theory and CASPT2 Energetics. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12792-12798. | 1.1 | 19 |
| 3655 | Stereostructure Assignment of Flexible Five-Membered Rings by GIAO ¹³ C NMR Calculations: Prediction of the Stereochemistry of Elatenyne. <i>Journal of Organic Chemistry</i> , 2008, 73, 4053-4062. | 1.7 | 82 |
| 3656 | Design and Synthesis of Propeller-Shaped Dispiroisoxazolinopiperidinochromanones. <i>ACS Combinatorial Science</i> , 2008, 10, 225-229. | 3.3 | 15 |
| 3657 | Palladium(II) and Platinum(II) Complexes with Heteroditopic 10-(Aryl)phenoxarsine (Aryl =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tff 50 Crystallization of cis Isomers. <i>Inorganic Chemistry</i> , 2008, 47, 1524-1531. | 1.9 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3658 | Assessment of the Accuracy of Density Functionals for Prediction of Relative Energies and Geometries of Low-Lying Isomers of Water Hexamers. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3976-3984. | 1.1 | 142 |
| 3659 | Pre-catalyst resting states: a kinetic, thermodynamic and quantum mechanical analyses of [PdCl ₂ (2-oxazoline) ₂] complexes. <i>Dalton Transactions</i> , 2008, , 3115. | 1.6 | 19 |
| 3660 | Bis(phosphanyl-amino)benzene ligands: a zinc(ii) complex and an unusual nickel(i) complex with a Dewar-benzene-type Ni ₂ P ₂ N ₂ backbone. <i>Dalton Transactions</i> , 2008, , 3107. | 1.6 | 13 |
| 3661 | Dependence of charge transfer reorganization energy on carrier localisation in organic molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 121-127. | 1.3 | 43 |
| 3662 | Dyotropic rearrangement of $\hat{1}^{\pm}$ -lactone to $\hat{1}^2$ -lactone: a computational study of small-ring halolactonisation. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 66-72. | 1.5 | 18 |
| 3663 | Dynamics and magnetic resonance properties of Sc ₃ C ₂ @C ₈₀ and its monoanion. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 7158. | 1.3 | 31 |
| 3664 | The intermolecular potential in NO ⁺ N ₂ and (NO ⁺ N ₂) ⁺ systems: implications for the neutralization of ionic molecular aggregates. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 5993. | 1.3 | 34 |
| 3665 | Alkali metal complexes of a naphthylamine-substituted phosphanide. <i>Dalton Transactions</i> , 2008, , 363-370. | 1.6 | 8 |
| 3666 | The reaction mechanism for the high quantum yield of Cypridina (Vargula) bioluminescence supported by the chemiluminescence of 6-aryl-2-methylimidazo[1,2-a]pyrazin-3(7H)-ones (Cypridina luciferin) <i>Tj ETQq0 0 0 rg BT/Overlook 10 Tf 50</i> | 1.6 | 10 |
| 3667 | A multi-technique approach to predicting the molecular structure of cuprizone in the gas phase and in the crystalline state. <i>CrystEngComm</i> , 2008, , . | 1.3 | 2 |
| 3668 | Supermolecule density functional calculations on the water exchange of aquated Al(iii) species in aqueous solution. <i>Chemical Communications</i> , 2008, , 3930. | 2.2 | 32 |
| 3669 | Polynitrogen/Nanoaluminum Surface Interactions. , 2008, , . | | 0 |
| 3670 | Design of Energetic Ionic Liquids. , 2008, , . | | 6 |
| 3671 | Influence of surface configurations of adsorbed cyanide ions to anodic dissolution of silver and gold in cyanide electrolytes. , 2008, , . | | 0 |
| 3672 | A computational analysis of the interaction between flavin and thiol(ate) groups. Implications for flavoenzyme catalysis. <i>Journal of Sulfur Chemistry</i> , 2008, 29, 415-424. | 1.0 | 6 |
| 3673 | A computational study of the intramolecular deprotonation of a carbon acid in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2475. | 1.3 | 8 |
| 3674 | Desorption electrospray ionization reactions between host crown ethers and the influenza neuraminidase inhibitor oseltamivir for the rapid screening of Tamiflu [®] . <i>Analyst, The</i> , 2008, 133, 1513. | 1.7 | 40 |
| 3675 | Electron density controlled carbamate ligand binding mode: towards a better understanding of metalloenzyme activity. <i>Dalton Transactions</i> , 2008, , 1821. | 1.6 | 8 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3676 | A new five-coordinated CuIP2NO2 system: XRD structure of 6-acetyl-1,3,7-trimethyl-pteridine-2,4(1H,3H)-dione and its Cu(i) (N5,O61,O4)-tridentate complex with triphenylphosphine. An AIM study of the nature of metal-ligand bonds. Dalton Transactions, 2008, , 6461. | 1.6 | 12 |
| 3677 | Ï€-Bonding versus oligomerisation in the aromatic anions [C6H4N2E]âˆ’: formation of the cyclic tetrameric tetraanion [C6H4N2Sb]44âˆ’ . Dalton Transactions, 2008, , 997-999. | 1.6 | 7 |
| 3678 | Promotion of phosphalkyne cyclooligomerisation by a Sb(v) to Sb(iii) redox process. Dalton Transactions, 2008, , 3753. | 1.6 | 10 |
| 3679 | Performance of multi-configurational calculations for a 1,4-bis(phenylethynyl)benzene derivative conjugated molecule. Physical Chemistry Chemical Physics, 2008, 10, 2308. | 1.3 | 4 |
| 3680 | Molecular Modeling of Complex Chemical Systems. Journal of the American Chemical Society, 2008, 130, 16824-16827. | 6.6 | 58 |
| 3681 | Is the FeO₂^{âˆ’} Anion Bent or Linear?. Journal of Physical Chemistry A, 2008, 112, 13641-13649. | 1.1 | 22 |
| 3682 | Rhodium-Catalyzed Câˆ’C Coupling Reactions: Mechanistic Considerations. Organometallics, 2008, 27, 4758-4771. | 1.1 | 39 |
| 3683 | Local correlation domains for coupled cluster theory: optical rotation and magnetic-field perturbations. Physical Chemistry Chemical Physics, 2008, 10, 3345. | 1.3 | 39 |
| 3684 | Boron di- and tri-cations. Dalton Transactions, 2008, , 6421. | 1.6 | 46 |
| 3685 | Direct synthesis of the 1,2,3-[Cî€6H4Pîf±Pîf±Pî€]âˆ’ anion, isoelectronic with the indenyl anion [Cî€6H4CHîf±CHîf±Cî€H]âˆ’ _{2.2} _{2.5} . Chemical Communications, 2008, , 859. | | |
| 3686 | Isolation of the first Li/halogen phosphinidenoid transition-metal complex. Dalton Transactions, 2008, , 2674. | 1.6 | 33 |
| 3687 | Ultrafast dynamics in thiophene investigated by femtosecond pump probe photoelectron spectroscopy and theory. Physical Chemistry Chemical Physics, 2008, 10, 393-404. | 1.3 | 50 |
| 3688 | The effects of self-aggregation on the vibrational circular dichroism and optical rotation measurements of glycidol. Physical Chemistry Chemical Physics, 2008, 10, 6787. | 1.3 | 30 |
| 3689 | Agostic-Type Bâˆ’Hâˆ’-Pb Interactions Stabilize a Dialkylplumblyene. Structure of and Bonding in [{<i>n</i>Pr₂P(BH₃)}(Me₃Si)C(CH₂)]₂Pb. Organometallics, 2008, 27, 4386-4394. | 1.1 | 25 |
| 3690 | Potent <i>s-cis</i>-Locked Bithiazole Correctors of Î”F508 Cystic Fibrosis Transmembrane Conductance Regulator Cellular Processing for Cystic Fibrosis Therapy. Journal of Medicinal Chemistry, 2008, 51, 6044-6054. | 2.9 | 49 |
| 3691 | Fragment-Localized Kohnâˆ’Sham Orbitals via a Singles Configuration-Interaction Procedure and Application to Local Properties and Intermolecular Energy Decomposition Analysis. Journal of Chemical Theory and Computation, 2008, 4, 2020-2029. | 2.3 | 51 |
| 3692 | Optical Properties of (GaAs)_{<i>n</i>} Clusters (<i>n</i> = 2âˆ’16). Journal of Physical Chemistry A, 2008, 112, 10728-10735. | 1.1 | 31 |
| 3693 | Biomimetic Asymmetric Total Synthesis of (âˆ’)-Laurefucin via an Organoselenium-Mediated Intramolecular Hydroxyetherification. Journal of the American Chemical Society, 2008, 130, 16807-16811. | 6.6 | 53 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3694 | Combined Experimental and Theoretical Study of the Mechanism and Enantioselectivity of Palladium-Catalyzed Intermolecular Heck Coupling. <i>Journal of the American Chemical Society</i> , 2008, 130, 10414-10421. | 6.6 | 97 |
| 3695 | Photophysical Studies of the Trans to Cis Isomerization of the Push-Pull Molecule: 1-(Pyridin-4-yl)-2-(N-methylpyrrol-2-yl)ethene (mepepy). <i>Journal of Physical Chemistry A</i> , 2008, 112, 8310-8315. | 1.1 | 9 |
| 3696 | Interplay among Tetrahedrane, Butterfly Diradical, and Planar Rhombus Structures in the Chemistry of the Binuclear Iron Carbonyl Phosphinidene Complexes Fe ₂ (CO) ₆ (PX) ₂ . <i>Journal of the American Chemical Society</i> , 2008, 130, 901-906. | 6.6 | 6 |
| 3697 | Reaction Rates and Dissolution Mechanisms of Quartz as a Function of pH. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2027-2033. | 1.1 | 101 |
| 3698 | Tuning the Redox Properties of Manganese(II) and Its Implications to the Electrochemistry of Manganese and Iron Superoxide Dismutases. <i>Inorganic Chemistry</i> , 2008, 47, 2897-2908. | 1.9 | 61 |
| 3699 | Range Separation and Local Hybridization in Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12530-12542. | 1.1 | 94 |
| 3700 | Ion-Pairing of Octyl Viologen Diiodide in Low-Polar Solvents: An Experimental and Computational Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7987-7995. | 1.1 | 26 |
| 3701 | Charge Transport in Single Au Alkanedithiol Au Junctions: Coordination Geometries and Conformational Degrees of Freedom. <i>Journal of the American Chemical Society</i> , 2008, 130, 318-326. | 6.6 | 464 |
| 3702 | Theoretical Survey of the Potential Energy Surface of Methyl Nitrite + Cu ⁺ Reaction. <i>Journal of Physical Chemistry A</i> , 2008, 112, 533-541. | 1.1 | 2 |
| 3703 | The Facile Generation of a Tetramethyleneethane Type Radical Cation and Biradical Utilizing a 3,4-Di(1-styryl)furan and a Photoinduced ET and Back ET Sequence. <i>Journal of the American Chemical Society</i> , 2008, 130, 2466-2472. | 6.6 | 12 |
| 3704 | Oriental Order of Difluorinated Liquid Crystals: A Comparative ¹³ C-NMR, Optical, and Dielectric Study in Nematic and Smectic B Phases. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9663-9676. | 1.2 | 27 |
| 3705 | Infrared Spectroscopy of [XF ₂ FeC ₂₄ H ₁₂] ⁺ (X = Tj, ET, Q, l, 1, 0.784314, rg, BT, /Overlock, 10, Tf, 50, 3, 12). Phase: Experimental and Computational Studies of Astrophysical Interest. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8551-8560. | 1.1 | 37 |
| 3706 | Understanding the Higher Reactivity of B ₂ cat ₂ versus B ₂ pin ₂ in Copper(I)-Catalyzed Alkene Diboration Reactions. <i>Organometallics</i> , 2008, 27, 1178-1186. | 1.1 | 108 |
| 3707 | On the Nature of the CP Bond in Phosphaalkynes. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 397-403. | 2.3 | 16 |
| 3708 | Electrostatically Embedded Many-Body Expansion for Simulations. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1-6. | 2.3 | 89 |
| 3709 | Influence of the Ligand Structure of Hafnocene Polymerization Catalysts: A Theoretical Study on Ethene Insertion and Chain Propagation. <i>Organometallics</i> , 2008, 27, 3390-3398. | 1.1 | 23 |
| 3710 | On the Electronic Structure and Chemical Bonding in the Tantalum Trimer Cluster. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10962-10967. | 1.1 | 47 |
| 3711 | Mechanism on Two-Electron Oxidation of Ubiquinol at the Q _p Site in Cytochrome <i>bc₁</i> Complex: B3LYP Study with Broken Symmetry. <i>Journal of Physical Chemistry B</i> , 2008, 112, 15116-15126. | 1.2 | 15 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3712 | The role of lone pairs in the chemical bonding of bare post-transition element clusters: the Wade-Mingos rules versus the jellium model. <i>Dalton Transactions</i> , 2008, , 6083. | 1.6 | 38 |
| 3713 | Bonding in Low-Coordinate Environments: Electronic Structure of Distorted Square-Planar Iron-Imido Complexes With Pincer-Type Ligands. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1576-1584. | 2.3 | 3 |
| 3714 | Theoretical Study on the Gas-Phase Acidity of Multiple Sites of Cu ⁺ Adenine and Cu ²⁺ Adenine Complexes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7418-7425. | 1.1 | 22 |
| 3715 | Ozonolysis of Geraniol-trans, 6-Methyl-5-hepten-2-one, and 6-Hydroxy-4-methyl-4-hexenal: Kinetics and Mechanisms. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6636-6645. | 1.1 | 12 |
| 3716 | Density Functional and Basis Set Dependence of Hydrated Ln(III) Properties. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 708-718. | 2.3 | 53 |
| 3717 | First Dinuclear B(II) Monocations with Bridging Guanidinate Ligands: Synthesis and Properties. <i>Inorganic Chemistry</i> , 2008, 47, 4774-4778. | 1.9 | 36 |
| 3718 | Calculation of One-Photon and Two-Photon Absorption Spectra of Porphyrins Using Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1094-1106. | 2.3 | 27 |
| 3719 | The HSSS Radical and the HSSS ⁻ Anion. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8471-8477. | 1.1 | 12 |
| 3720 | Jacobsen's Catalyst Interaction with Polydimethylsiloxane/Tetraethoxysilane Network and Solvent Molecules: Theoretical Design of a New Polymeric Membrane. <i>Journal of Physical Chemistry C</i> , 2008, 112, 14830-14834. | 1.5 | 9 |
| 3721 | A Theoretical Study of the Cyclization Processes of Energized CCCSi and CCCP. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12714-12720. | 1.1 | 6 |
| 3722 | Po(IV) Hydration: A Quantum Chemical Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5416-5422. | 1.2 | 21 |
| 3723 | Multireference Model Chemistries for Thermochemical Kinetics. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1208-1219. | 2.3 | 131 |
| 3724 | Characterization of the Switch in the Mechanism of an Intramolecular Diels-Alder Reaction. <i>Journal of Organic Chemistry</i> , 2008, 73, 467-473. | 1.7 | 14 |
| 3725 | Computational Study of Iron Bis(dithiolene) Complexes: Redox Non-Innocent Ligands and Antiferromagnetic Coupling. <i>Inorganic Chemistry</i> , 2008, 47, 10037-10045. | 1.9 | 16 |
| 3726 | Chapter 6 Structure of Isolated Clusters. <i>Handbook of Metal Physics</i> , 2008, 5, 143-173. | 0.0 | 1 |
| 3727 | Interaction of CO with PdAu(111) and PdAu(100) Bimetallic Surfaces: A Theoretical Cluster Model Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6073-6081. | 1.5 | 36 |
| 3728 | Modeling the Vibronic Spectra of Transition Metal Complexes: The Ligand-Field Spectrum of [PtCl ₄] ²⁻ . <i>Inorganic Chemistry</i> , 2008, 47, 4817-4825. | 1.9 | 10 |
| 3729 | Quantum Chemical Study of Lewis Acid Catalyzed Allylboration of Aldehydes. <i>Journal of the American Chemical Society</i> , 2008, 130, 12519-12526. | 6.6 | 53 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3730 | Excitation Energies from Spin-Restricted Ensemble-Referenced Kohn-Sham Method: A State-Average Approach. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12980-12988. | 1.1 | 55 |
| 3731 | Relativistic Model Core Potential Study of the Au+Xe System. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5236-5242. | 1.1 | 23 |
| 3732 | Spin States at a Tipping Point: What Determines the d ² Ground State of Nickel(III) Tetra(<i>i</i> -butyl)porphyrin Dicyanide?. <i>Journal of Physical Chemistry B</i> , 2008, 112, 1053-1056. | 1.2 | 15 |
| 3733 | Degenerate Perturbation Theory for Electronic g Tensors: Leading-Order Relativistic Effects. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1810-1828. | 2.3 | 20 |
| 3734 | Multicoefficient Density Functional Theory (MC-DFT). <i>Journal of Physical Chemistry A</i> , 2008, 112, 1064-1070. | 1.1 | 7 |
| 3735 | High-Stability Hydrogenated Silicon-Carbon Clusters: A Full Study of Si ₂ C ₂ H ₂ in Comparison to Si ₂ C ₂ , C ₂ B ₂ H ₄ , and Other Similar Species. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5712-5719. | 1.1 | 22 |
| 3736 | From Fullerenes and Icosahedral Diamondoids to Polyicosahedral Nanowires: Structural, Electronic, and Mechanical Characteristics. <i>Journal of Physical Chemistry C</i> , 2008, 112, 11122-11129. | 1.5 | 12 |
| 3737 | A Heterobimetallic Complex With an Unsupported Uranium(III)-Aluminum(I) Bond: (CpSiMe ₃) ₃ U-AlCp* (Cp* = C ₅ Me ₅). <i>Journal of the American Chemical Society</i> , 2008, 130, 10086-10087. | 6.6 | 112 |
| 3738 | Hierarchical Self-Assembly of Aminopyrazole Peptides into Nanorosettes in Water. <i>Journal of the American Chemical Society</i> , 2008, 130, 586-591. | 6.6 | 20 |
| 3739 | Accurate Molecular Polarizabilities Based on Continuum Electrostatics. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1480-1493. | 2.3 | 18 |
| 3740 | Theoretical Study of the Phototoxicity of Naproxen and the Active Form of Nabumetone. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10921-10930. | 1.1 | 21 |
| 3741 | Structural and Electronic Characteristics of Diamondoid Analogues of Group 14 Elements. <i>Journal of Physical Chemistry C</i> , 2008, 112, 16324-16330. | 1.5 | 14 |
| 3742 | Modified Carbon Pseudopotential for Use in ONIOM Calculations of Alkyl-Substituted Metallocenes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12754-12760. | 1.1 | 11 |
| 3743 | Theoretical Studies on Synthetic and Biosynthetic Oxidopyrylium-Alkene Cycloadditions: Pericyclic Pathways to Intricarene. <i>Journal of Organic Chemistry</i> , 2008, 73, 1516-1523. | 1.7 | 47 |
| 3744 | Regioselective Ortho Palladation of Stabilized Iminophosphoranes in Exo Positions: Scope, Limitations, and Mechanistic Insights. <i>Organometallics</i> , 2008, 27, 2929-2936. | 1.1 | 41 |
| 3745 | Benchmark Data for Interactions in Zeolite Model Complexes and Their Use for Assessment and Validation of Electronic Structure Methods. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6860-6868. | 1.5 | 157 |
| 3746 | Structural Investigation of Encapsulated Fluoride in Polyhedral Oligomeric Silsesquioxane Cages Using Ion Mobility Mass Spectrometry and Molecular Mechanics. <i>Chemistry of Materials</i> , 2008, 20, 4299-4309. | 3.2 | 82 |
| 3747 | Rotational Reorientation Dynamics of Oxazine 750 in Polar Solvents. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3646-3655. | 1.1 | 20 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3748 | Toward Calculations of the ¹²⁹ Xe Chemical Shift in Xe@C ₆₀ at Experimental Conditions: Relativity, Correlation, and Dynamics. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2658-2668. | 1.1 | 60 |
| 3749 | Mechanistic Insights into the Stereocontrolled Synthesis of Hexahydropyrrolo[2,3-b]indoles by Electrophilic Activation of Tryptophan Derivatives. <i>Organic Letters</i> , 2008, 10, 77-80. | 2.4 | 81 |
| 3750 | Structural and Dielectric Properties of Quartz-Water Interfaces. <i>Journal of Physical Chemistry C</i> , 2008, 112, 19986-19994. | 1.5 | 67 |
| 3751 | Assessment of a Middle-Range Hybrid Functional. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1254-1262. | 2.3 | 155 |
| 3752 | Where Does the Electron Go? Electron Distribution and Reactivity of Peptide Cation Radicals Formed by Electron Transfer in the Gas phase. <i>Journal of the American Chemical Society</i> , 2008, 130, 8818-8833. | 6.6 | 60 |
| 3753 | Local Hybrid Divide-and-Conquer Method for the Computation of Medium and Large Molecules. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 2049-2056. | 2.3 | 6 |
| 3754 | Ions Related to Silynes and Disilynes: Computational Studies. <i>Organometallics</i> , 2008, 27, 1707-1715. | 1.1 | 17 |
| 3755 | DFT Study on Chemical N ₂ Fixation by Using a Cubane-Type Ru ₃ S ₄ Cluster: Energy Profile for Binding and Reduction of N ₂ to Ammonia via Ru ^{II} N ^{III} NH ₂ (<i>x</i> = 1-3) Intermediates with Unique Structures. <i>Journal of the American Chemical Society</i> , 2008, 130, 9037-9047. | 6.6 | 49 |
| 3756 | Theoretical Investigation of the Fe ⁺ -Catalyzed Oxidation of Acetylene by N ₂ O. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5676-5683. | 1.1 | 29 |
| 3757 | New Insights into the Use of (TD-)DFT for Geometries and Electronic Structures of Constrained π -Stacked Systems: [<i>n</i> . <i>n</i>]Paracyclophanes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13691-13698. | 1.1 | 18 |
| 3758 | Theoretical Analysis of the Mechanism for the Oxidative Carbonylation of Toluene to <i>p</i> -Toluic Acid by Rhodium Complexes. <i>Journal of Physical Chemistry C</i> , 2008, 112, 2129-2136. | 1.5 | 16 |
| 3759 | Assessment of New Meta and Hybrid Meta Density Functionals for Predicting the Geometry and Binding Energy of a Challenging System: The Dimer of H ₂ S and Benzene. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6009-6016. | 1.1 | 33 |
| 3760 | Nuclear Magnetic Shielding of the ¹¹³ Cd(II) Ion in Aqua Solution: A Combined Molecular Dynamics/Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 11347-11352. | 1.2 | 7 |
| 3761 | Spectroscopic Signatures of Nitrogen-Substituted Zeolites. <i>Journal of the American Chemical Society</i> , 2008, 130, 14912-14913. | 6.6 | 33 |
| 3762 | Synthesis and Structure of Organoantimony(III) Compounds Containing Antimony-Selenium and -Tellurium Terminal Bonds. <i>Organometallics</i> , 2008, 27, 6059-6062. | 1.1 | 44 |
| 3763 | Understanding the Highly Regioselective Cyanothiolation of 1-Alkynes Catalyzed by Palladium Phosphine Complexes. <i>Organometallics</i> , 2008, 27, 246-253. | 1.1 | 43 |
| 3764 | Synthesizability of the Heavy Analogues of Disubstituted Cyclopropenylidene: A Theoretical Study. <i>Organometallics</i> , 2008, 27, 5571-5576. | 1.1 | 10 |
| 3765 | Computational Study of the Gas Phase Reactions of Isopropylimido and Allylimido Tungsten Precursors for Chemical Vapor Deposition of Tungsten Carbonitride Films: Implications for the Choice of Carrier Gas. <i>Chemistry of Materials</i> , 2008, 20, 7246-7251. | 3.2 | 21 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3766 | Prediction of a New Pathway to Presilphiperfolanol. <i>Organic Letters</i> , 2008, 10, 4827-4830. | 2.4 | 49 |
| 3767 | Analytic Calculations of Vibrational Hyperpolarizabilities in the Atomic Orbital Basis. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11942-11950. | 1.1 | 30 |
| 3768 | DFT Study of the Products, Potential Energy Surface, and Substituent Effects for Methyl Radical Addition to $[\text{Rh}(\text{PMe}_3)_2(\text{CO})\text{X}]$ (X = Halogen or CN). <i>Organometallics</i> , 2008, 27, 2004-2012. | 1.1 | 11 |
| 3769 | DFT Studies on the Mechanism of the Diboration of Aldehydes Catalyzed by Copper(I) Boryl Complexes. <i>Journal of the American Chemical Society</i> , 2008, 130, 5586-5594. | 6.6 | 193 |
| 3770 | Structure and Vibrational Dynamics of Model Compounds of the $[\text{FeFe}]^{\text{H}}$ Hydrogenase Enzyme System via Ultrafast Two-Dimensional Infrared Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10023-10032. | 1.2 | 41 |
| 3771 | Theoretical Investigation of the Mechanism of Acid-Catalyzed Oxygenation of a Pd(II)-Hydride To Produce a Pd(II)-Hydroperoxide. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1283-1292. | 2.3 | 21 |
| 3772 | Computational Density Functional Study of Polypyrrrolic Macrocycles: Analysis of Actinyl-Oxo to 3d Transition Metal Bonding. <i>Inorganic Chemistry</i> , 2008, 47, 11583-11592. | 1.9 | 35 |
| 3773 | Rational Design of Macrometalloccyclic Trinuclear Complexes with Superior pK_a -Acidity and pK_b -Basicity. <i>Journal of the American Chemical Society</i> , 2008, 130, 1669-1675. | 6.6 | 107 |
| 3774 | The ketene intermediate in the photochemistry of ortho-nitrobenzaldehyde. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 3872. | 1.3 | 55 |
| 3775 | Redox Transformations of Bis(2,2'-bipyridine)(1-methyl-1-pyridin-2-yl-ethylamine)ruthenium(II). <i>Inorganic Chemistry</i> , 2008, 47, 5314-5323. | 1.9 | 5 |
| 3776 | Dependence of Charge-Transport Parameters on Static Correlation and Self-Interaction Energy: The Case of a 1,4-Bis(Phenylethynyl)Benzene Derivative Conjugated Molecule. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10325-10332. | 1.1 | 22 |
| 3777 | Microhydration of the Guanine-Cytosine (GC) Base Pair in the Neutral and Anionic Radical States: A Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5189-5198. | 1.2 | 48 |
| 3778 | Oxygen-Centered Hexatantalum Tetradecaimido Cluster Complexes. <i>Inorganic Chemistry</i> , 2008, 47, 1053-1066. | 1.9 | 20 |
| 3779 | Beyond the Wade-Mingos Rules in Bare 10- and 12-Vertex Germanium Clusters: Transition States for Symmetry Breaking Processes. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 209-215. | 2.3 | 8 |
| 3780 | Experimental Evidence for an Inverse Hydrogen Migration in Arginine Radicals. <i>Journal of the American Chemical Society</i> , 2008, 130, 7645-7654. | 6.6 | 35 |
| 3781 | Synthesis and Structure of a Ferrocenylboron Dication. <i>Inorganic Chemistry</i> , 2008, 47, 7456-7458. | 1.9 | 36 |
| 3782 | Relation between the pK_a -Contribution to Reversed Si-C Bond Polarization and the Reaction Profile for the Thermolytic Formation of Silenes. <i>Organometallics</i> , 2008, 27, 5203-5211. | 1.1 | 15 |
| 3783 | Theoretical Study of the Orientation Rules in Photonnucleophilic Aromatic Substitutions. <i>Journal of Organic Chemistry</i> , 2008, 73, 1243-1252. | 1.7 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3784 | Absorption Spectra of Blue-Light-Emitting Oligoquinolines from Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2008, 112, 13701-13710. | 1.2 | 10 |
| 3785 | Theoretical Studies on Coupling Reactions of Carbon Dioxide with Alkynes Mediated by Nickel(0) Complexes. <i>Organometallics</i> , 2008, 27, 3892-3900. | 1.1 | 45 |
| 3786 | Further Shortening of the C-C Single Bond in Substituted Tetrahedranyl Tetrahedrane Systems: An Energy Decomposition Analysis. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12919-12924. | 1.1 | 9 |
| 3787 | Semiempirical Double-Hybrid Density Functional with Improved Description of Long-Range Correlation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2702-2712. | 1.1 | 123 |
| 3788 | Electronic, Optical, and Vibrational Properties of Bridged Dithienylethylene-Based NLO Chromophores. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3109-3120. | 1.5 | 48 |
| 3789 | Mechanistic Studies on Fast Ligand Substitution Reactions of Pt(II) in Different Ionic Liquids: Role of Solvent Polarity and Ion-Pair Formation. <i>Inorganic Chemistry</i> , 2008, 47, 7121-7132. | 1.9 | 28 |
| 3790 | Quantitative Three Dimensional Structure Linear Interaction Energy Model of 5'-O-(N-(Salicyl)sulfamoyl]adenosine and the Aryl Acid Adenylating Enzyme MbtA. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 7154-7160. | 2.9 | 21 |
| 3791 | Mechanism for Iron-Catalyzed Alkene Isomerization in Solution. <i>Organometallics</i> , 2008, 27, 4370-4379. | 1.1 | 44 |
| 3792 | Spin-Orbit and Electron Correlation Effects on the Structure of EF ₃ (E = I, At, and) Tj ETQq0 0 0 rgBT, /Overlock 10 Tf 50 4 | 1.2 | 15 |
| 3793 | Hidden Histidine Radical Rearrangements upon Electron Transfer to Gas-Phase Peptide Ions. Experimental Evidence and Theoretical Analysis. <i>Journal of the American Chemical Society</i> , 2008, 130, 14584-14596. | 6.6 | 64 |
| 3794 | Theoretical Study of the Mechanism and Rate Constant of the B + CO ₂ Reaction. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8148-8153. | 1.1 | 3 |
| 3795 | Allenyl Azide Cycloaddition Chemistry: Exploration of the Scope and Mechanism of Cyclopentenelated Dihydropyrrole Synthesis through Azatrimethylenemethane Intermediates. <i>Journal of Organic Chemistry</i> , 2008, 73, 5090-5099. | 1.7 | 25 |
| 3796 | Structural Correspondences between the Low-Energy Nanoclusters of Silica and Water. <i>Journal of Physical Chemistry C</i> , 2008, 112, 18417-18425. | 1.5 | 7 |
| 3797 | Free Radical Conformations and Conversions in X-Irradiated Single Crystals of α -Cysteic Acid by Electron Magnetic Resonance and Density Functional Theory Studies. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4284-4293. | 1.1 | 4 |
| 3798 | Charge-Transfer-Based Mechanism for Half-Metallicity and Ferromagnetism in One-Dimensional Organometallic Sandwich Molecular Wires. <i>Journal of the American Chemical Society</i> , 2008, 130, 13956-13960. | 6.6 | 118 |
| 3799 | Improved Description of Stereoelectronic Effects in Hydrocarbons Using Semilocal Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 888-891. | 2.3 | 63 |
| 3800 | Initial Hardness Response and Hardness Profiles in the Study of Woodward-Hoffmann Rules for Electrocyclizations. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 595-602. | 2.3 | 51 |
| 3801 | Electrochemical, Magnetic, and Electrical Properties of β -Capped Sexithiophene Films. Part 3. Conduction in Poly(bis-terthienyl-B)s (B = Ethane, Disulfide, Diacetylene, Acetylene, Ethylene). <i>Chemistry of Materials</i> , 2008, 20, 6847-6856. | 3.2 | 12 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3802 | The Boron Connection: A Parallel Description of Aromatic, Bonding, and Structural Characteristics of Hydrogenated Silicon-Carbon Clusters and Isovalent Carboranes. <i>Inorganic Chemistry</i> , 2008, 47, 8823-8829. | 1.9 | 17 |
| 3803 | Theoretical Studies on O-Insertion Reactions of Nitrous Oxide with Ruthenium Hydride Complexes. <i>Organometallics</i> , 2008, 27, 3825-3833. | 1.1 | 35 |
| 3804 | Mechanism of Thiolate-Disulfide Interchange Reactions in Biochemistry. <i>Journal of Organic Chemistry</i> , 2008, 73, 12-21. | 1.7 | 124 |
| 3805 | Formation of Sugar Radicals in RNA Model Systems and Oligomers via Excitation of Guanine Cation Radical. <i>Journal of Physical Chemistry B</i> , 2008, 112, 2168-2178. | 1.2 | 33 |
| 3806 | Highly Efficient Pyridylpyrazole Ligands for the Heck Reaction. A Combined Experimental and Computational Study. <i>Organometallics</i> , 2008, 27, 1084-1091. | 1.1 | 57 |
| 3807 | Performance of DFT Methods in the Calculation of Optical Spectra of Chromophores. , 2008, , . | | 1 |
| 3808 | Valence Electronic Structure of Benzo-2,1,3-chalcogenadiazoles Studied by Photoelectron Spectroscopy and Density Functional Theory. <i>Inorganic Chemistry</i> , 2008, 47, 6220-6226. | 1.9 | 35 |
| 3809 | One-Electron Metal-Metal Bond Stabilized in Dinuclear Metallocenes: Theoretical Prediction of DBe-LiCp (D = C ₅ H ₅ or C ₅ Me ₅). <i>Journal of Physical Chemistry A</i> , 2008, 112, 12463-12468. | 1.1 | 9 |
| 3810 | Addition of Alkyl Radicals to Transition-Metal-Coordinated CO: Calculation of the Reaction of [Ru(CO) ₅] and Related Complexes and Relevance to Alkane Carbonylation. <i>Journal of the American Chemical Society</i> , 2008, 130, 511-521. | 6.6 | 22 |
| 3811 | A Combined Spectroscopic and Theoretical Study of Dibutyltin Diacetate and Dilaurate in Supercritical CO ₂ . <i>Journal of Physical Chemistry A</i> , 2008, 112, 8379-8386. | 1.1 | 10 |
| 3812 | Chemisorption-induced Structural Changes and Transition from Chemisorption to Physisorption in Au ₆ (CO) _n (n = 4-9). <i>Journal of Physical Chemistry C</i> , 2008, 112, 11920-11928. | 1.5 | 51 |
| 3813 | Surface Reaction of 1,2-Dichloroethylene on Si(100)-2 × 1: Importance of Surface Isomerization Channel. <i>Journal of Physical Chemistry C</i> , 2008, 112, 9327-9335. | 1.5 | 7 |
| 3814 | On the Origin of Diastereoselectivity in [2 + 2 + 2] Cycloisomerization of Chiral Triynes: Controlling Helicity of Helicene-like Compounds by Thermodynamic Factors. <i>Journal of Organic Chemistry</i> , 2008, 73, 2074-2082. | 1.7 | 75 |
| 3815 | The pDynamo Program for Molecular Simulations using Hybrid Quantum Chemical and Molecular Mechanical Potentials. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1151-1161. | 2.3 | 99 |
| 3816 | The Acidity and Proton Affinity of the Damaged Base 1,6-Ethnoadenine in the Gas Phase versus in Solution: Intrinsic Reactivity and Biological Implications. <i>Journal of Organic Chemistry</i> , 2008, 73, 5907-5914. | 1.7 | 34 |
| 3817 | 1,5-Anti Stereocontrol in the Boron-Mediated Aldol Reactions of ¹² -Alkoxy Methyl Ketones: The Role of the Formyl Hydrogen Bond. <i>Journal of Organic Chemistry</i> , 2008, 73, 1253-1263. | 1.7 | 65 |
| 3818 | Octacoordinate Carbons Encaged Inside Carborane Clusters: A Density Functional Theory Investigation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7643-7651. | 1.1 | 2 |
| 3819 | Biophysical Techniques in Photosynthesis. <i>Advances in Photosynthesis and Respiration</i> , 2008, , . | 1.0 | 21 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3820 | Density functional study of Bi ₂ Te ₃ and Bi ₄ Te ₆ molecules. <i>Molecular Physics</i> , 2008, 106, 2699-2708. | 0.8 | 0 |
| 3821 | Parameters For Excess Electron Transfer in DNA. Estimation Using Unoccupied Kohn-Sham Orbitals and TD DFT. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9043-9049. | 1.1 | 20 |
| 3822 | First-Principles Determination of Molecular Conformations of Cyclic Adenosine 3',5'-Monophosphate in Gas Phase and Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16851-16859. | 1.2 | 4 |
| 3823 | FT-IR, FT-Raman spectra and DFT vibrational analysis of 2-aminobiphenyl. <i>Molecular Simulation</i> , 2008, 34, 277-287. | 0.9 | 13 |
| 3824 | When Arsenic Makes the Difference: Chelating Phosphino and Bridging Arsenoarylthiolato Gallium Complexes. <i>Inorganic Chemistry</i> , 2008, 47, 11284-11293. | 1.9 | 21 |
| 3825 | Coordination Properties of Lysine Interacting with Co(I) and Co(II). A Theoretical and Mass Spectrometry Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12385-12392. | 1.1 | 9 |
| 3826 | Gas-Phase Thermochemical Properties of Pyrimidine Nucleobases. <i>Journal of Organic Chemistry</i> , 2008, 73, 9283-9291. | 1.7 | 59 |
| 3827 | Computational Prediction of Absorbance Maxima for a Structurally Diverse Series of Engineered Green Fluorescent Protein Chromophores. <i>Journal of Physical Chemistry B</i> , 2008, 112, 2533-2541. | 1.2 | 29 |
| 3828 | Inhibition of Siderophore Biosynthesis in <i>Mycobacterium tuberculosis</i> with Nucleoside Bisubstrate Analogues: Structure-Activity Relationships of the Nucleobase Domain of 5'-O-(Salicyl)sulfamoyl]adenosine. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 5349-5370. | 2.9 | 118 |
| 3829 | Molecular Recognition at Methyl Methacrylate/n-Butyl Acrylate (MMA/nBA) Monomer Unit Boundaries of Phospholipids at p-MMA/nBA Copolymer Surfaces. <i>Langmuir</i> , 2008, 24, 10382-10389. | 1.6 | 9 |
| 3830 | M ₂ @C ₇₉ N (M = Y, Tb): Isolation and Characterization of Stable Endohedral Metallofullerenes Exhibiting M-M Bonding Interactions inside Aza[80]fullerene Cages. <i>Journal of the American Chemical Society</i> , 2008, 130, 12992-12997. | 6.6 | 155 |
| 3831 | Theoretical Analysis of the Hydrogen-Transfer Reaction to C-N, C-C, and C-C Bonds Catalyzed by Shvo's Ruthenium Complex. <i>Organometallics</i> , 2008, 27, 4854-4863. | 1.1 | 44 |
| 3832 | Modeling the Photophysics and Photochromic Potential of 1,2-Dihydronaphthalene (DHN): A Combined CASPT2/CASSCF-Topological and MMVB-Dynamical Investigation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10096-10107. | 1.1 | 14 |
| 3833 | Changes in the Isotropic Shielding of the ¹⁷ O Nucleus upon Torsion in Terminal Oxygen Systems: A Computational Study on Their Origin. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9118-9127. | 1.1 | 4 |
| 3834 | Theoretical Study of the Gas-Phase Chemiionization Reactions La + O and La + O ₂ . <i>Journal of Physical Chemistry A</i> , 2008, 112, 7825-7830. | 1.1 | 19 |
| 3835 | first principles Study of the Reaction of Formic and Acetic Acids with Hydroxyl Radicals. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6918-6928. | 1.1 | 20 |
| 3836 | Halogen Bonding with Dihalogens and Interhalogens. , 2007, , 65-104. | | 59 |
| 3837 | First-principles-derived kinetics of the reactions involved in low-temperature dimethyl ether oxidation. <i>Molecular Physics</i> , 2008, 106, 367-396. | 0.8 | 27 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3838 | A new parameter-free correlation functional based on an average atomic reduced density gradient analysis. <i>Journal of Chemical Physics</i> , 2008, 128, 034101. | 1.2 | 56 |
| 3839 | Low-lying isomers of the B ₉ boron cluster: The planar molecular wheel versus three-dimensional structures. <i>Journal of Chemical Physics</i> , 2008, 129, 024302. | 1.2 | 82 |
| 3840 | A THEORETICAL INVESTIGATION OF MECHANISM OF THE ADENOSINE DEAMINASE MODIFICATION: REACTION OF GLUTAMATE RESIDUE WITH WOODWARD REAGENT K. <i>Journal of Theoretical and Computational Chemistry</i> , 2008, 07, 1121-1145. | 1.8 | 1 |
| 3841 | ELECTRONIC AND STERIC MECHANISMS IN MONO- AND DOUBLE-FLUORINATION OF Cs-C ₆₀ Cl ₆ . <i>Modern Physics Letters B</i> , 2008, 22, 2727-2738. | 1.0 | 3 |
| 3842 | Lactic acid in solution: Investigations of lactic acid self-aggregation and hydrogen bonding interactions with water and methanol using vibrational absorption and vibrational circular dichroism spectroscopies. <i>Journal of Chemical Physics</i> , 2008, 128, 014508. | 1.2 | 95 |
| 3843 | High-efficiency, low-voltage phosphorescent organic light-emitting diode devices with mixed host. <i>Journal of Applied Physics</i> , 2008, 104, . | 1.1 | 143 |
| 3844 | Singlet and Triplet Methylene (CH ₂) Plus P ₄ : A Computational Study. <i>Organometallics</i> , 2008, 27, 3399-3402. | 1.1 | 15 |
| 3845 | Reliability of range-separated hybrid functionals for describing magnetic coupling in molecular systems. <i>Journal of Chemical Physics</i> , 2008, 129, 184110. | 1.2 | 74 |
| 3846 | A hybrid explicit/implicit solvation method for first-principle molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2008, 128, 144501. | 1.2 | 79 |
| 3847 | Complex polarization propagator calculations of magnetic circular dichroism spectra. <i>Journal of Chemical Physics</i> , 2008, 128, 094103. | 1.2 | 63 |
| 3848 | Eliminating spin contamination in auxiliary-field quantum Monte Carlo: Realistic potential energy curve of F ₂ . <i>Journal of Chemical Physics</i> , 2008, 128, 114309. | 1.2 | 53 |
| 3849 | What can we learn from the adiabatic connection formalism about local hybrid functionals?. <i>Journal of Chemical Physics</i> , 2008, 128, 214107. | 1.2 | 44 |
| 3850 | Current through single conjugated molecules: Calculations versus measurements. <i>Journal of Chemical Physics</i> , 2008, 129, 024901. | 1.2 | 8 |
| 3851 | Adiabatic connection forms in density functional theory: H ₂ and the He isoelectronic series. <i>Journal of Chemical Physics</i> , 2008, 129, 064105. | 1.2 | 21 |
| 3852 | Tungsten carbide revisited: New anion photoelectron spectrum and density functional theory calculations. <i>Journal of Chemical Physics</i> , 2008, 129, 114304. | 1.2 | 16 |
| 3853 | Self-consistent generalized Kohn-Sham local hybrid functionals of screened exchange: Combining local and range-separated hybridization. <i>Journal of Chemical Physics</i> , 2008, 129, 124110. | 1.2 | 68 |
| 3854 | Analytical calculations of frequency-dependent hypermagnetizabilities and Cotton-Mouton constants using London atomic orbitals. <i>Journal of Chemical Physics</i> , 2008, 129, 164110. | 1.2 | 23 |
| 3855 | Selective calculation of high-intensity vibrations in molecular resonance Raman spectra. <i>Journal of Chemical Physics</i> , 2008, 129, 204103. | 1.2 | 36 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3857 | Regulation of Bestrophin Cl Channels by Calcium: Role of the C Terminus. <i>Journal of General Physiology</i> , 2008, 132, 681-692. | 0.9 | 74 |
| 3858 | Mechanism of thermal decomposition of carbamoyl phosphate and its stabilization by aspartate and ornithine transcarbamoylases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 16918-16923. | 3.3 | 25 |
| 3859 | Terahertz spectroscopic investigation of L-glutamic acid and L-tyrosine. <i>Measurement Science and Technology</i> , 2008, 19, 015602. | 1.4 | 20 |
| 3860 | Density functional study of double ionization energies. <i>Journal of Chemical Physics</i> , 2008, 128, 084112. | 1.2 | 11 |
| 3861 | Ab initio spectroscopy and photoinduced cooling of the trans-stilbene molecule. <i>Journal of Chemical Physics</i> , 2008, 128, 164303. | 1.2 | 75 |
| 3862 | A new class of silicon-carbon clusters: A full study of the hydrogenated $\text{Si}_n\text{C}_2\text{H}_2$, $n=3,4,5$, clusters in comparison with their isoelectronic carboranes $\text{C}_2\text{B}_n\text{H}_{n+2}$. <i>Journal of Chemical Physics</i> , 2008, 128, 184305. | 1.2 | 15 |
| 3863 | Hartree-Fock orbitals significantly improve the reaction barrier heights predicted by semilocal density functionals. <i>Journal of Chemical Physics</i> , 2008, 128, 244112. | 1.2 | 89 |
| 3864 | Good performance of the M06 family of hybrid meta generalized gradient approximation density functionals on a difficult case: CO adsorption on $\text{MgO}(001)$. <i>Journal of Chemical Physics</i> , 2008, 129, 124710. | 1.2 | 90 |
| 3865 | Effect of microstructure on deprotection kinetics in photoresist. <i>Journal of Vacuum Science & Technology B</i> , 2008, 26, 2311-2315. | 1.3 | 0 |
| 3866 | Are Octahedral Ruthenium(II/III) and Osmium(II/III) Complexes Always Low-Spin?. <i>Collection of Czechoslovak Chemical Communications</i> , 2008, 73, 1231-1244. | 1.0 | 0 |
| 3867 | Electronic structure and lattice vibrations of $\text{Ca}_2\text{CuO}_2\text{Cl}_2$: A hybrid density functional study. <i>Physical Review B</i> , 2008, 77, . | 1.1 | 3 |
| 3868 | High-symmetry low-energy structures of $\text{C}_{60}\text{H}_{60}$ and related fullerenes and nanotubes. <i>Physical Review B</i> , 2008, 77, . | 1.1 | 18 |
| 3869 | Substituent effects on the hydrogen-bonded complex of aniline-H ₂ O: a computational study. <i>New Journal of Chemistry</i> , 2008, 32, 1060. | 1.4 | 17 |
| 3870 | Exploring the High Pressure Phase Diagrams of Light Elements Using Large Scale Ab-initio Molecular Dynamics Simulations. 2008 22nd International Symposium on High Performance Computing Systems and Applications, 2008, . | 0.0 | 0 |
| 3871 | Performance of the M06 family of exchange-correlation functionals for predicting magnetic coupling in organic and inorganic molecules. <i>Journal of Chemical Physics</i> , 2008, 128, 114103. | 1.2 | 208 |
| 3872 | Photoabsorption spectra of small fullerenes and Si-heterofullerenes. <i>Journal of Chemical Physics</i> , 2008, 128, 154307. | 1.2 | 22 |
| 3873 | Syntheses, characterization, spectroscopy, and quantum chemical calculation of two 2-(N-2-aminopyridyl)pyridinium salts: observation of an acyclic water pentamer. <i>Journal of Coordination Chemistry</i> , 2008, 61, 1088-1101. | 0.8 | 3 |
| 3874 | First-principles calculation of the O vacancy in ZnO: A self-consistent gap-corrected approach. <i>Physical Review B</i> , 2008, 77, . | 1.1 | 137 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3875 | The augmented Roothaan-Hall method for optimizing Hartree-Fock and Kohn-Sham density matrices. <i>Journal of Chemical Physics</i> , 2008, 129, 124106. | 1.2 | 45 |
| 3876 | Theoretical Description of the Geometry, Electronic Structure and Reactivity Analysis for a Set of <i>Tris</i> -Chelates with Application in Organic Light Emitting Diodes. <i>Journal of the Chinese Chemical Society</i> , 2008, 55, 535-542. | 0.8 | 1 |
| 3877 | Computational Study on the Existence of Organic Peroxy Radical-Water Complexes (RO ₂ -H ₂ O). <i>Journal of Physical Chemistry A</i> , 2008, 112, 1587-1595. | 1.1 | 36 |
| 3878 | The Infrared Spectra of Very Large, Compact, Highly Symmetric, Polycyclic Aromatic Hydrocarbons (PAHs). <i>Astrophysical Journal</i> , 2008, 678, 316-327. | 1.6 | 165 |
| 3879 | The restricted active space followed by second-order perturbation theory method: Theory and application to the study of CuO ₂ and Cu ₂ O ₂ systems. <i>Journal of Chemical Physics</i> , 2008, 128, 204109. | 1.2 | 430 |
| 3880 | Copper Complexes of Nicotinic-Aromatic Carboxylic Acids as Superoxide Dismutase Mimetics. <i>Molecules</i> , 2008, 13, 3040-3056. | 1.7 | 79 |
| 3882 | Evaluation of group electronegativities and hardness (softness) of group 14 elements and containing functional groups through density functional theory and correlation with NMR spectra data. <i>Eletica Quimica</i> , 2008, 33, 69-76. | 0.2 | 11 |
| 3883 | A DFT Study on Deactivation of Triplet Excited State Riboflavin by Polyphenols. <i>International Journal of Molecular Sciences</i> , 2008, 9, 1908-1914. | 1.8 | 9 |
| 3884 | THE 5.25 AND 5.7 μ m ASTRONOMICAL POLYCYCLIC AROMATIC HYDROCARBON EMISSION FEATURES. <i>Astrophysical Journal</i> , 2009, 690, 1208-1221. | 1.6 | 48 |
| 3886 | Three New Spongian Diterpenes from the Fijian Marine Sponge <i>Spongia</i> sp. <i>Natural Product Communications</i> , 2009, 4, 1934578X0900400. | 0.2 | 6 |
| 3887 | THE FAR-INFRARED EMISSION FROM THE Mg ⁺⁺ -PAH SPECIES. <i>Astrophysical Journal</i> , 2009, 698, 275-280. | 1.6 | 18 |
| 3888 | Experimental magnetic form factors in $\langle \text{Co} \rangle$ A combined study of <i>ab initio</i> calculations, magnetic Compton scattering, and polarized neutron diffraction. <i>Physical Review B</i> , 2009, 79, . | 1.1 | 16 |
| 3889 | Description of magnetic interactions in strongly correlated solids via range-separated hybrid functionals. <i>Physical Review B</i> , 2009, 79, . | 1.1 | 44 |
| 3890 | Structures of Mo _x W(3 \tilde{x})O ₆ ^($\chi=3$) anion and neutral clusters determined by anion photoelectron spectroscopy and density functional theory calculations. <i>Journal of Chemical Physics</i> , 2009, 131, 044310. | 1.2 | 32 |
| 3891 | Bonding between the cesium cation and substituted benzoic acids or benzoate anions in the gas phase: A density functional theory and mass spectrometric study. <i>Collection of Czechoslovak Chemical Communications</i> , 2009, 74, 167-188. | 1.0 | 8 |
| 3892 | Role of noncollinear magnetization for the first-order electric-dipole hyperpolarizability at the four-component Kohn-Sham density functional theory level. <i>Journal of Chemical Physics</i> , 2009, 130, 024109. | 1.2 | 14 |
| 3893 | Efficient computation of the dispersion interaction with density-functional theory. <i>Physical Review A</i> , 2009, 79, . | 1.0 | 53 |
| 3894 | Density functional estimations of Heisenberg exchange constants in oligonuclear magnetic compounds: Assessment of density functional theory versus <i>ab initio</i> . <i>Journal of Chemical Physics</i> , 2009, 131, 224316. | 1.2 | 15 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3895 | Strong-field phase-dependent molecular dissociation. <i>Physical Review A</i> , 2009, 79, . | 1.0 | 27 |
| 3896 | Gas phase and bulk ultraviolet photoemission spectroscopy of 3,4,9,10-perylene-tetracarboxylic dianhydride, 1,4,5,8-naphthalene-tetracarboxylic dianhydride, and 1,8-naphthalene-dicarboxylic anhydride. <i>Journal of Chemical Physics</i> , 2009, 131, 034711. | 1.2 | 29 |
| 3897 | Fluorescence quenching in an organic donor-acceptor dyad: A first principles study. <i>Journal of Chemical Physics</i> , 2009, 131, 034310. | 1.2 | 15 |
| 3898 | Fe ⁺ and Mg ⁺ -polycyclic aromatic hydrocarbon complexes. <i>Molecular Physics</i> , 2009, 107, 809-818. | 0.8 | 12 |
| 3899 | Prediction of excitation energies for conjugated polymers using time-dependent density functional theory. <i>Physical Review B</i> , 2009, 80, . | 1.1 | 12 |
| 3900 | Stabilization of large silicon fullerenes and related nanostructures through puckering and poly(oligo)merization. <i>Physical Review B</i> , 2009, 80, . | 1.1 | 20 |
| 3901 | Density functional method including weak interactions: Dispersion coefficients based on the local response approximation. <i>Journal of Chemical Physics</i> , 2009, 131, 224104. | 1.2 | 204 |
| 3902 | Photoabsorption spectra of small cationic xenon clusters from time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2009, 131, 214302. | 1.2 | 4 |
| 3903 | A new all-round density functional based on spin states and S _N 2 barriers. <i>Journal of Chemical Physics</i> , 2009, 131, 094103. | 1.2 | 113 |
| 3904 | Vibrational coupled cluster theory with full two-mode and approximate three-mode couplings: The VCC[2pt3] model. <i>Journal of Chemical Physics</i> , 2009, 131, 034115. | 1.2 | 29 |
| 3905 | Rationalizing and functionalizing stannaspherene: Very stable stannaspherene "alloys". <i>Journal of Chemical Physics</i> , 2009, 131, 224310. | 1.2 | 21 |
| 3906 | Success and pitfalls of the Sin ² C2H2=C2Bn ² Hn isolobal analogy: Depth and breadth of the boron connection. <i>Journal of Chemical Physics</i> , 2009, 130, 064303. | 1.2 | 13 |
| 3907 | Endohedral Cluster of Li ₁₀ O with T _d Symmetry. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13451-13456. | 1.1 | 3 |
| 3908 | Spectroscopic Studies of the Light-Color Modulation Mechanism of Firefly (Beetle) Bioluminescence. <i>Journal of the American Chemical Society</i> , 2009, 131, 2385-2396. | 6.6 | 133 |
| 3909 | exo-Substituent effects in halogenated icosahedral (B ₁₂ H ₁₂) and octahedral (B ₆ H ₆) closo-borane skeletons: chemical reactivity studied by experimental and quantum chemical methods. <i>Collection of Czechoslovak Chemical Communications</i> , 2009, 74, 1-27. | 1.0 | 16 |
| 3910 | Physical Image vs. Structure Relation, Part 131: Computational Evidences for the 2h J PH Spin Spin Coupling in Internally H-Bonded Isomers of Some 1-Oxoalkanephosphonate Hydrazones. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2009, 184, 1036-1046. | 0.8 | 8 |
| 3912 | A relook at the compliance constants in redundant internal coordinates and some new insights. <i>Journal of Chemical Physics</i> , 2009, 131, 174112. | 1.2 | 25 |
| 3913 | An insight into the structure of model germaphosphaallenes. <i>Molecular Physics</i> , 2009, 107, 1161-1167. | 0.8 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3914 | SOLVENT AND SUBSTITUENT EFFECTS ON THE INTRAMOLECULAR AMIDE HYDROLYSIS OF N-METHYLMALAMIC ACID. <i>Journal of Theoretical and Computational Chemistry</i> , 2009, 08, 1217-1226. | 1.8 | 1 |
| 3915 | Optical activity in conformationally flexible molecules: a theoretical study of large-amplitude vibrational averaging in (<i>R</i>)-3-chloro-1-butene. <i>Molecular Physics</i> , 2009, 107, 1041-1057. | 0.8 | 32 |
| 3917 | Doping of TiO_2 for Altered Optical and Photocatalytic Properties. <i>International Journal of Photoenergy</i> , 2009, 2009, 1-22. | 1.4 | 65 |
| 3918 | Post-CCSD(T) ab Initio Thermochemistry of Halogen Oxides and Related Hydrides XOX , XOOX , HOX , XO_n , and HXO_n ($X = \text{F}, \text{Cl}$), and Evaluation of DFT Methods for These Systems. <i>Journal of Physical Chemistry A</i> , 2009, 113, 4802-4816. | 1.1 | 77 |
| 3919 | A quantum chemistry study of Diels-Alder dimerizations in benzene and anthracene. <i>Journal of Chemical Physics</i> , 2009, 131, 024313. | 1.2 | 16 |
| 3920 | Review of Hierarchical Multiscale Modeling to Describe the Mechanical Behavior of Amorphous Polymers. <i>Journal of Engineering Materials and Technology, Transactions of the ASME</i> , 2009, 131, . | 0.8 | 65 |
| 3921 | Mixed donor-functionalised phosphinomethanide complexes of the alkali metals; synthesis, structures, and solution dynamics. <i>Dalton Transactions</i> , 2009, , 6159. | 1.6 | 8 |
| 3922 | Theoretical investigation of the water/corundum (0001) interface. <i>Journal of Chemical Physics</i> , 2009, 130, 064702. | 1.2 | 15 |
| 3923 | Ab initio thermochemistry using optimal-balance models withisodesmic corrections: The ATOMIC protocol. <i>Journal of Chemical Physics</i> , 2009, 130, 144113. | 1.2 | 29 |
| 3924 | Benchmarking density-functional-theory calculations of rotational g tensors and magnetizabilities using accurate coupled-cluster calculations. <i>Journal of Chemical Physics</i> , 2009, 131, 144104. | 1.2 | 60 |
| 3925 | Local hybrids as a perturbation to global hybrid functionals. <i>Journal of Chemical Physics</i> , 2009, 131, 154112. | 1.2 | 33 |
| 3926 | Using circumacenes to improve organic electronics and molecular electronics: design clues. <i>Nanotechnology</i> , 2009, 20, 475201. | 1.3 | 9 |
| 3927 | Theoretical Study on Reactions of Triplet Excited State Thioxanthone with Indole. <i>International Journal of Molecular Sciences</i> , 2009, 10, 4284-4289. | 1.8 | 9 |
| 3928 | Mechanism of Action of Cyclophilin A Explored by Metadynamics Simulations. <i>PLoS Computational Biology</i> , 2009, 5, e1000309. | 1.5 | 43 |
| 3929 | Numerical evaluation of electron repulsion integrals for pseudoatomic orbitals and their derivatives. <i>Journal of Chemical Physics</i> , 2009, 130, 124114. | 1.2 | 13 |
| 3930 | Calculating electron paramagnetic resonance g -matrices for triplet state molecules from multireference spin-orbit configuration interaction wave functions. <i>Journal of Chemical Physics</i> , 2009, 130, 154106. | 1.2 | 14 |
| 3931 | An accurate density functional theory calculation for electronic excitation energies: The least-squares support vector machine. <i>Journal of Chemical Physics</i> , 2009, 130, 184104. | 1.2 | 20 |
| 3932 | Development and assessment of a short-range meta-GGA functional. <i>Journal of Chemical Physics</i> , 2009, 130, 234112. | 1.2 | 48 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 3933 | Multiple coherent states for first-principles semiclassical initial value representation molecular dynamics. <i>Journal of Chemical Physics</i> , 2009, 130, 234113. | 1.2 | 82 |
| 3934 | Adsorption of O ₂ on Cobalt(II) Pyrrole Molecules from First-Principles Calculations. <i>Journal of the Physical Society of Japan</i> , 2009, 78, 094710. | 0.7 | 16 |
| 3935 | FAR-INFRARED SPECTROSCOPY OF NEUTRAL CORONENE, OVALENE, AND DICORONYLENE. <i>Astronomical Journal</i> , 2009, 137, 4054-4060. | 1.9 | 36 |
| 3936 | An organometallic route to long helicenes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 13169-13174. | 3.3 | 126 |
| 3937 | Electronic and Vibrational Circular Dichroism Spectra of Chiral 4-X-[2.2]paracyclophanes with X Containing Fluorine Atoms. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14851-14859. | 1.1 | 13 |
| 3938 | Dramatic Influence of the Electronic Structure on the Conductivity through Open and Closed Shell Molecules. <i>Advanced Materials</i> , 2009, 21, 1177-1181. | 11.1 | 45 |
| 3939 | Precise Structure of Pentacene Monolayers on Amorphous Silicon Oxide and Relation to Charge Transport. <i>Advanced Materials</i> , 2009, 21, 2294-2298. | 11.1 | 183 |
| 3940 | An N-Linked Bidentate Phosphoramidite Ligand (N-Me-BIPAM) for Rhodium-Catalyzed Asymmetric Addition of Arylboronic Acids to N-Sulfonylaldimines. <i>Advanced Synthesis and Catalysis</i> , 2009, 351, 260-270. | 2.1 | 82 |
| 3942 | Synthesis, chiroptical properties, and their theoretical simulation of some highly rotating benzo-tricamphor derivatives. <i>Chirality</i> , 2009, 21, E86-97. | 1.3 | 10 |
| 3943 | Comparative Analysis of Electron Density and Electron Localization Function for Dinuclear Manganese Complexes with Bridging Boron and Carbon-Centered Ligands. <i>Chemistry - A European Journal</i> , 2009, 15, 623-632. | 1.7 | 38 |
| 3944 | The Effect of a Complexed Lithium Cation on a Norcaradiene-Based Radical Clock. <i>Chemistry - A European Journal</i> , 2009, 15, 2425-2433. | 1.7 | 7 |
| 3945 | Oriental Properties of Poly(<i>n</i> -benzyl-L-glutamate): Influence of Molecular Weight and Solvent on Order Parameters of the Solute. <i>Chemistry - A European Journal</i> , 2009, 15, 254-260. | 1.7 | 78 |
| 3946 | Macrocyclic Cyclooctene-Supported AlCl ₃ -Salen Catalysts for Conjugated Addition Reactions: Effect of Linker and Support Structure on Catalysis. <i>Chemistry - A European Journal</i> , 2009, 15, 1186-1194. | 1.7 | 29 |
| 3947 | Rainbow Perylene Monoimides: Easy Control of Optical Properties. <i>Chemistry - A European Journal</i> , 2009, 15, 878-884. | 1.7 | 79 |
| 3948 | Thiophene-Diazine Molecular Semiconductors: Synthesis, Structural, Electrochemical, Optical, and Electronic Structural Properties; Implementation in Organic Field-Effect Transistors. <i>Chemistry - A European Journal</i> , 2009, 15, 5023-5039. | 1.7 | 82 |
| 3949 | A Stable Six-Coordinate Intermediate in Ammonia-Dinitrogen Exchange at Schrock's Molybdenum Catalyst. <i>Chemistry - A European Journal</i> , 2009, 15, 5073-5082. | 1.7 | 50 |
| 3950 | Rhodium(I)-Catalysed Intramolecular [2+2+2] Cyclotrimerisations of 15-, 20- and 25-Membered Azamacrocycles: Experimental and Theoretical Mechanistic Studies. <i>Chemistry - A European Journal</i> , 2009, 15, 5289-5300. | 1.7 | 49 |
| 3951 | Bonding or Nonbonding? Description or Explanation? σ -Confinement Bonding of He@adamantane. <i>Chemistry - A European Journal</i> , 2009, 15, 6032-6040. | 1.7 | 30 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 3952 | Synthesis and Properties of Salen ²⁺ Aluminum Complexes as a Novel Class of Color-Tunable Luminophores. <i>Chemistry - A European Journal</i> , 2009, 15, 6478-6487. | 1.7 | 56 |
| 3953 | A New Generation of Anticancer Drugs: Mesoporous Materials Modified with Titanocene Complexes. <i>Chemistry - A European Journal</i> , 2009, 15, 5588-5597. | 1.7 | 79 |
| 3954 | Oxidation of End-Capped Pentathienoacenes and Characterization of Their Radical Cations. <i>Chemistry - A European Journal</i> , 2009, 15, 12346-12361. | 1.7 | 17 |
| 3955 | Polyamine Receptors Containing Dipyridine or Phenanthroline Units: Clues for the Design of Fluorescent Chemosensors for Metal Ions. <i>Chemistry - A European Journal</i> , 2009, 15, 8049-8063. | 1.7 | 27 |
| 3956 | Synthesis and EPR Studies of 2'-Deoxyuridines with Alkynyl, Rodlike Linkages. <i>Chemistry - A European Journal</i> , 2009, 15, 7569-7577. | 1.7 | 15 |
| 3957 | Synthesis, Structure, and Bonding of Novel Homodinuclear Cobalt and Nickel Borylene Complexes. <i>Chemistry - A European Journal</i> , 2009, 15, 7150-7155. | 1.7 | 11 |
| 3958 | Synthesis, Spectroscopy, Nonlinear Optics, and Theoretical Investigations of Thienylethynyl Octopoles with a Tunable Core. <i>Chemistry - A European Journal</i> , 2009, 15, 8223-8234. | 1.7 | 14 |
| 3959 | Interfacial Impregnation Chemistry in the Synthesis of Cobalt Catalysts Supported on Titania. <i>Chemistry - A European Journal</i> , 2009, 15, 13090-13104. | 1.7 | 23 |
| 3960 | From Mono- to Poly-Substituted Frameworks: A Way of Tuning the Acidic Character of C ₃ H in <i>o</i> -Carborane Derivatives. <i>Chemistry - A European Journal</i> , 2009, 15, 9755-9763. | 1.7 | 43 |
| 3961 | Do Extremely Bent Allenes Exist?. <i>Chemistry - A European Journal</i> , 2009, 15, 7287-7291. | 1.7 | 70 |
| 3962 | Brønsted Acid Catalyzed Morita-Baylis-Hillman Reaction: A New Mechanistic View for Thioureas Revealed by ESI-MS(/MS) Monitoring and DFT Calculations. <i>Chemistry - A European Journal</i> , 2009, 15, 12460-12469. | 1.7 | 72 |
| 3963 | UF ₆ and UF ₄ in Liquid Ammonia: [UF ₇ (NH ₃) ³⁺] and [UF ₄ (NH ₃) ₄]. <i>Chemistry - A European Journal</i> , 2009, 15, 8269-8274. | 1.7 | 21 |
| 3964 | Synthesis, Structure, Photoluminescence and Photoreactivity of 2,3-Diphenyl-4-neopentyl-1-silacyclobut-2-enes. <i>Chemistry - A European Journal</i> , 2009, 15, 8625-8645. | 1.7 | 13 |
| 3965 | Cycloaddition Reactions of Butadiene and 1,3-Dipoles to Curved Arenes, Fullerenes, and Nanotubes: Theoretical Evaluation of the Role of Distortion Energies on Activation Barriers. <i>Chemistry - A European Journal</i> , 2009, 15, 13219-13231. | 1.7 | 92 |
| 3966 | Geminal Ionic Liquids: A Combined Approach to Investigate Their Three-Dimensional Organisation. <i>Chemistry - A European Journal</i> , 2009, 15, 13059-13068. | 1.7 | 27 |
| 3967 | Nickel-Catalyzed Cross-Coupling of Alkyl Zinc Halides for the Formation of C(sp ²) ₂ -C(sp ³) Bonds: Scope and Mechanism. <i>Chemistry - A European Journal</i> , 2009, 15, 12681-12688. | 1.7 | 90 |
| 3968 | Energy Transport along Conjugated Polymer Chains with Extended Radiative Lifetimes: A Theoretical Study. <i>ChemPhysChem</i> , 2009, 10, 3061-3068. | 1.0 | 7 |
| 3969 | FT Raman and DFT Study on a Series of All-anti Oligothienoacenes End-Capped with Triisopropylsilyl Groups. <i>ChemPhysChem</i> , 2009, 10, 3069-3076. | 1.0 | 11 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3970 | Isotropic ¹³ C Hyperfine Coupling Constants Distinguish Neutral from Anionic Ubiquinone-Derived Radicals. <i>ChemPhysChem</i> , 2009, 10, 3187-3189. | 1.0 | 7 |
| 3971 | Hydron-Transfer Processes Involving an Organotitanium Oxide and Alcohols. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 643-653. | 1.0 | 13 |
| 3972 | Equilibrium and Kinetic Studies of the Reactions between Aqua[1-(2-aminoethyl)piperazine]palladium(II) and Biologically Relevant Nucleophiles. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 2261-2270. | 1.0 | 29 |
| 3973 | Controlling Selectivity for Cycloadditions of Nitrones and Alkenes Tethered by Benzimidazoles: Combining Experiment and Theory. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 1578-1584. | 1.2 | 10 |
| 3974 | Synthesis and Photophysical Characterisation of Fluorescent 8-(1 <i>H</i> -1,2,3-Triazol-4-yl)adenosine Derivatives. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 1515-1521. | 1.2 | 48 |
| 3975 | Intramolecular Nonbonded Interactions Between Divalent Selenium Centers with Donor and Acceptor Substituents. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 2765-2774. | 1.2 | 17 |
| 3976 | Karplus-Type Dependence of Vicinal ¹¹⁹ Sn- ¹³ C and ¹¹⁹ Sn- ¹ H Spin-Spin Couplings in Organotin(IV) Derivatives: A DFT Study. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 3526-3534. | 1.2 | 14 |
| 3977 | Triphenylamine-Based Pyridine <i>N</i> -Oxide and Pyridinium Salts for Size-Selective Recognition of Dicarboxylates. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 4515-4524. | 1.2 | 45 |
| 3978 | Conformational Analysis and Optical Rotation of Carene ¹² Amino Alcohols: A DFT Study. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 4600-4605. | 1.2 | 9 |
| 3979 | Synthesis of (±) Wine Lactone and Its Analogues by a Diels-Alder Approach. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 4405-4411. | 1.2 | 9 |
| 3980 | Synthesis of Prolines by Enantioselective 1,3-Dipolar Cycloaddition of Azomethine Ylides and Alkenes Catalyzed by Chiral Phosphoramidite-Silver(I) Complexes. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 5622-5634. | 1.2 | 61 |
| 3981 | On the Regioselective Intramolecular Nucleophilic Addition of Thiols to C ₆₀ . <i>European Journal of Organic Chemistry</i> , 2009, 2009, 6231-6238. | 1.2 | 16 |
| 3982 | Chemical bonding in view of electron charge density and kinetic energy density descriptors. <i>Journal of Computational Chemistry</i> , 2009, 30, 1093-1102. | 1.5 | 62 |
| 3983 | Accurate prediction of heats of formation by a combined method of B3LYP and neural network correction. <i>Journal of Computational Chemistry</i> , 2009, 30, 1424-1444. | 1.5 | 26 |
| 3984 | Crystal structure prediction of flexible molecules using parallel genetic algorithms with a standard force field. <i>Journal of Computational Chemistry</i> , 2009, 30, 1973-1985. | 1.5 | 29 |
| 3985 | Gibbs energy of activation for thermal isomerization of (1Z)-acetaldehyde hydrazone and (1Z)-acetaldehyde N,N-dimethylhydrazone by Gaussian-4 theory and CCSD(T)/CBS computations. <i>Journal of Computational Chemistry</i> , 2009, 30, 2176-2180. | 1.5 | 3 |
| 3986 | A stationary-wave model of enzyme catalysis. <i>Journal of Computational Chemistry</i> , 2010, 31, 343-350. | 1.5 | 6 |
| 3987 | Extension of QM/MM docking and its applications to metalloproteins. <i>Journal of Computational Chemistry</i> , 2009, 30, 2609-2616. | 1.5 | 62 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 3988 | The effect of the sixth sulfur ligand in the catalytic mechanism of periplasmic nitrate reductase. <i>Journal of Computational Chemistry</i> , 2009, 30, 2466-2484. | 1.5 | 48 |
| 3989 | Rate coefficients for the reaction of OH with CF ₃ CH ₂ CH ₃ (HFC-263fb) between 200 and 400 K: <i>Ab initio</i> , DFT, and transition state theory calculations. <i>Journal of Computational Chemistry</i> , 2010, 31, 500-509. | 1.5 | 9 |
| 3990 | Computational determination of fundamental pathway and activation barriers for acetohydroxyacid synthase-catalyzed condensation reactions of α -keto acids. <i>Journal of Computational Chemistry</i> , 2010, 31, 1592-1602. | 1.5 | 19 |
| 3991 | Covalent hydration energies for purine analogs by quantum chemical methods. <i>Journal of Computational Chemistry</i> , 2010, 31, 721-725. | 1.5 | 6 |
| 3992 | Using electronic polarization from the internal continuum (EPIC) for intermolecular interactions. <i>Journal of Computational Chemistry</i> , 2010, 31, 811-824. | 1.5 | 8 |
| 3993 | On the use of symmetry in the <i>ab initio</i> quantum mechanical simulation of nanotubes and related materials. <i>Journal of Computational Chemistry</i> , 2010, 31, 855-862. | 1.5 | 48 |
| 3994 | Interaction energy and the shift in OH stretch frequency on hydrogen bonding for the H ₂ O...H ₂ O, CH ₃ OH...H ₂ O, and H ₂ O...CH ₃ OH dimers. <i>Journal of Computational Chemistry</i> , 2010, 31, 963-972. | 1.5 | 17 |
| 3995 | Evaluation of exchange-correlation functionals for time-dependent density functional theory calculations on metal complexes. <i>Journal of Computational Chemistry</i> , 2010, 31, 1008-1014. | 1.5 | 27 |
| 3996 | How the choice of a computational model could rule the chemical interpretation: The Ni(II) catalyzed ethylene dimerization as a case study. <i>Journal of Computational Chemistry</i> , 2010, 31, 1053-1062. | 1.5 | 8 |
| 3997 | Intramolecular electronic communication in a dimethylaminoazobenzene-fullerene C ₆₀ dyad: An experimental and TD-DFT study. <i>Journal of Computational Chemistry</i> , 2010, 31, 1182-1194. | 1.5 | 8 |
| 3998 | Barrier heights for H-atom abstraction by H ₂ from <i>n</i> -butanol: A simple yet exacting test for model chemistries?. <i>Journal of Computational Chemistry</i> , 2010, 31, 1236-1248. | 1.5 | 80 |
| 3999 | Spatial structure and NMR spectra of strained [2.2.2]cyclophanes. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, 407-414. | 1.1 | 5 |
| 4000 | Theoretical investigation on multinuclear NMR chemical shifts of some tris(trifluoromethyl)boron complexes. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, 629-634. | 1.1 | 3 |
| 4001 | How different are diastereomorphous orientations of enantiomers in the liquid crystalline phases of PBLG and PBDG: a case study. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, 734-740. | 1.1 | 37 |
| 4002 | Structure determination of slowly exchanging conformers in solution using high-resolution NMR, computational modeling and DFT GIAO chemical shielding: application to an erythronolide A derivative. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, 909-916. | 1.1 | 6 |
| 4003 | DFT simulations and Vibrational spectra of 4-chloro and 4-bromophenylboronic acid molecules. <i>Journal of Raman Spectroscopy</i> , 2009, 40, 67-75. | 1.2 | 49 |
| 4004 | The intramolecular charge transfer in a donor-acceptor dianion probed by resonance Raman spectroscopy and quantum chemical calculations. <i>Journal of Raman Spectroscopy</i> , 2009, 40, 1158-1161. | 1.2 | 4 |
| 4005 | FTIR, FT-Raman, and computational calculations of 4-chloro-(3-chlorophenyl carbamoyl)phenyl acetate. <i>Journal of Raman Spectroscopy</i> , 2009, 40, 2176-2186. | 1.2 | 27 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4006 | FTIR, FT-Raman, SERS spectra and computational calculations of 4-(2-hydroxy-5-nitrophenyl)benzamide. <i>Journal of Raman Spectroscopy</i> , 2010, 41, 381-390. | 1.2 | 6 |
| 4008 | When Do Interacting Atoms Form a Chemical Bond? Spectroscopic Measurements and Theoretical Analyses of Dideuteriophenanthrene. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 2592-2595. | 7.2 | 137 |
| 4009 | Hydrogen-Bonding Catalysts Based on Fluorinated Alcohol Derivatives for Living Polymerization. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 5170-5173. | 7.2 | 107 |
| 4010 | Synthesis and molecular structures of 1-chloro-1-silacyclopent-2-enes. Combination of 1,2-hydroboration, 1,1-organoboration and protodeborylation. <i>Applied Organometallic Chemistry</i> , 2009, 23, 124-131. | 1.7 | 18 |
| 4011 | Theoretical study of the hydroxylation of phenolates by the Cu ₂ O ₂ (N,N'-dimethylethylenediamine) ₂ 2+ complex. <i>Journal of Biological Inorganic Chemistry</i> , 2009, 14, 229-242. | 1.1 | 17 |
| 4012 | Theoretical studies on the molecular structure and vibrational spectra of some dimethyl substituted pyridine derivatives. <i>Journal of Molecular Modeling</i> , 2009, 15, 79-90. | 0.8 | 12 |
| 4013 | Systematic characterization on electronic structures and spectra for a series of complexes, M(IDB)Cl ₂ (M = Mn, Fe, Co, Ni, Cu and Zn): a theoretical study. <i>Journal of Molecular Modeling</i> , 2009, 15, 469-479. | 0.8 | 10 |
| 4014 | Theoretical study on the thermal decomposition of model compounds for Poly (dialkyl fumarate). <i>Journal of Molecular Modeling</i> , 2009, 15, 1043-1049. | 0.8 | 2 |
| 4015 | Catalytic activities of dismutation reactions of Cu(bpy)Br ₂ compound and its derivatives as SOD mimics: A theoretical study. <i>Journal of Molecular Modeling</i> , 2009, 15, 1397-1405. | 0.8 | 4 |
| 4016 | A quantum-chemical study on ion complexation in polymer electrolytes containing lithium aluminate salts. <i>Solid State Ionics</i> , 2009, 180, 934-940. | 1.3 | 2 |
| 4017 | A route to enantiomerically pure 5-(2-hydroxyethyl)cyclopent-2-en-1-ol and its absolute configuration by Mosher esters. <i>Tetrahedron: Asymmetry</i> , 2009, 20, 449-456. | 1.8 | 8 |
| 4018 | Carbocation rearrangements in aspernomine biosynthesis. <i>Tetrahedron Letters</i> , 2009, 50, 1578-1581. | 0.7 | 15 |
| 4019 | A theoretical insight into the deactivating reactions of triplet excited state C60 by \hat{I}^2 -carotene. <i>Computational and Theoretical Chemistry</i> , 2009, 893, 111-113. | 1.5 | 1 |
| 4020 | Substituent effects on the tautomerism of monochalcogenocarboxylic acids XC(O)YH (X=H, F, NH ₂). <i>Tetrahedron Letters</i> , 2009, 50, 896, 80-84. | 1.5 | 9 |
| 4021 | Oxidative damage to DNA: Theoretical determination of ionization potential of deoxyriboguanosine (dG) and deoxyribocytidine (dC) and proton transfer in its cation. <i>Computational and Theoretical Chemistry</i> , 2009, 909, 25-32. | 1.5 | 6 |
| 4022 | A full conformational space analysis of bilirubin. <i>Computational and Theoretical Chemistry</i> , 2009, 911, 24-29. | 1.5 | 8 |
| 4023 | Theoretical study of the scavenging mechanism to 1,4-dicarbonyls by pyridoxamine: The water-assisted reaction. <i>Computational and Theoretical Chemistry</i> , 2009, 911, 70-74. | 1.5 | 4 |
| 4024 | Theoretical study on the mechanism of nickel(0)-mediated coupling between carbon dioxide and epoxyethane. <i>Computational and Theoretical Chemistry</i> , 2009, 916, 125-134. | 1.5 | 26 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4025 | A molecule with small rotational constants containing an atom with a large nuclear quadrupole moment: The microwave spectrum of trans-1-iodoperfluoropropane. <i>Journal of Molecular Spectroscopy</i> , 2009, 257, 66-73. | 0.4 | 16 |
| 4026 | Halogenation effects of pheniramines on the complexation with β -cyclodextrin. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2009, 50, 392-396. | 1.4 | 14 |
| 4027 | Importance of hydrogen bonding for second harmonic generation effect: X-ray diffraction and DFT study on S-benzyl isothiuronium chloride. <i>Journal of Physics and Chemistry of Solids</i> , 2009, 70, 322-325. | 1.9 | 3 |
| 4028 | Oxidative transformations in the W/H ₂ O ₂ /RCOOH system. <i>Mendeleev Communications</i> , 2009, 19, 175-181. | 0.6 | 5 |
| 4029 | Theoretical investigation on the molecular structure, Infrared, Raman and NMR spectra of para-halogen benzenesulfonamides, 4-X-C ₆ H ₄ SO ₂ NH ₂ (X=Cl, Br or F). <i>Journal of Molecular Structure</i> , 2009, 919, 26-33. | 1.8 | 49 |
| 4030 | Experimental and theoretical study of the conformational, vibrational and magnetic properties of 4,6-di-O-acetyl-2,3-dideoxy-d-threo-hex-2-enopyranosyl ethanesulfonamide. <i>Journal of Molecular Structure</i> , 2009, 919, 223-226. | 1.8 | 5 |
| 4031 | Theoretical and experimental vibrational spectroscopic study of 3-piperidino-propylamine. <i>Journal of Molecular Structure</i> , 2009, 923, 120-126. | 1.8 | 19 |
| 4032 | Exploring rearrangements along the fragmentation pathways of diuron anion: A combined experimental and computational investigation. <i>International Journal of Mass Spectrometry</i> , 2009, 288, 6-15. | 0.7 | 13 |
| 4033 | Evidence of neutral radical induced analyte ion transformations in APPI and Near-VUV APLI. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 1868-1880. | 1.2 | 17 |
| 4034 | Conformational analysis of o-allylphenol by density functional and IR spectroscopy methods. <i>Journal of Applied Spectroscopy</i> , 2009, 76, 630-640. | 0.3 | 4 |
| 4035 | Testing the performance of density functionals for the calculation of energetic properties of complex-forming radical-molecule reactions. <i>Reaction Kinetics and Catalysis Letters</i> , 2009, 96, 233-244. | 0.6 | 4 |
| 4036 | Conformational in the IR spectra of 1-hydroxyethyl derivatives of 1,4-benzo-and 5,8-dihydroxy-1,4-naphthoquinones: A DFT study. <i>Russian Chemical Bulletin</i> , 2009, 58, 663-674. | 0.4 | 1 |
| 4037 | Structural and Kinetic DFT Characterization of Materials to Rationalize Catalytic Performance. <i>Topics in Catalysis</i> , 2009, 52, 444-455. | 1.3 | 11 |
| 4038 | A parallel study of Ni@Si ₁₂ and Cu@Si ₁₂ nanoclusters. <i>Journal of Mathematical Chemistry</i> , 2009, 46, 971-980. | 0.7 | 11 |
| 4039 | Mixed silicon-germanium nanocrystals: a detailed study of Si _x Ge _{47-x} :H. <i>Journal of Mathematical Chemistry</i> , 2009, 46, 942-951. | 0.7 | 5 |
| 4040 | Optical properties of ultra small Si nanoparticles: potential role of surface reconstruction and oxygen contamination. <i>Journal of Mathematical Chemistry</i> , 2009, 46, 952-961. | 0.7 | 6 |
| 4041 | Optical gap and excitation energies of small Ge nanocrystals. <i>Journal of Mathematical Chemistry</i> , 2009, 46, 934-941. | 0.7 | 8 |
| 4042 | Theoretical study on the reaction of CN radicals with ClO radicals by density functional theory. <i>Science in China Series B: Chemistry</i> , 2009, 52, 1973-1979. | 0.8 | 0 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4043 | A theoretical investigation of intermolecular interaction of a phthalimide based α -oxon α -off α -sensor with different halide ions: tuning its efficiency and electro-optical properties. Theoretical Chemistry Accounts, 2009, 122, 77-86. | 0.5 | 33 |
| 4044 | Activation enthalpies of pericyclic reactions: the performances of some recently proposed functionals. Theoretical Chemistry Accounts, 2009, 122, 257-264. | 0.5 | 16 |
| 4045 | Density functional methods in the study of oxygen transfer reactions. Theoretical Chemistry Accounts, 2009, 123, 59-66. | 0.5 | 3 |
| 4046 | Interaction between uracil nucleobase and phenylalanine amino acid: the role of sodium cation in stacking. Theoretical Chemistry Accounts, 2009, 124, 115-122. | 0.5 | 34 |
| 4047 | First-principles determination of molecular conformations of indolizidine ($\hat{\alpha}$)-235B $\hat{\alpha}$ ² in solution. Theoretical Chemistry Accounts, 2009, 124, 269-278. | 0.5 | 3 |
| 4048 | Density functional theory of transition metal phthalocyanines, II: $\hat{\alpha}$ electronic structure of MnPc and FePc $\hat{\alpha}$ symmetry and symmetry breaking. Applied Physics A: Materials Science and Processing, 2009, 95, 165-172. | 1.1 | 100 |
| 4049 | Density functional theory of transition metal phthalocyanines, I: $\hat{\alpha}$ electronic structure of NiPc and CoPc $\hat{\alpha}$ self-interaction effects. Applied Physics A: Materials Science and Processing, 2009, 95, 159-163. | 1.1 | 105 |
| 4050 | Thermophysical properties of the $\hat{\alpha}$ polymorphs of Mg ₂ SiO ₄ : a computational study. Physics and Chemistry of Minerals, 2009, 36, 87-106. | 0.3 | 44 |
| 4051 | Hydrogen Cyanide Exchange on [Al(HCN) ₆] ³⁺ $\hat{\alpha}$ A DFT Study. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2009, 635, 434-438. | 0.6 | 6 |
| 4052 | Syntheses, Crystal Structure and Reactivity of Tin(II) Bis[<i>N</i> -(diphenylphosphanyl)(2 $\hat{\alpha}$ pyridylmethyl)amide]. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2009, 635, 462-470. | 0.6 | 9 |
| 4053 | (Ph ₄ P) ₂ [Be ₃ ($\hat{\alpha}$ OH) ₃ (H ₂ O) ₆]Cl ₅ : Crystal Structure and DFT Calculations. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2009, 635, 1196-1199. | 0.6 | 14 |
| 4054 | Spectroscopy and DFT Calculations. First Observation of Isotope $\hat{\alpha}$ Induced Chemical Shifts ^{10/11} B(¹³ C), and the Signs and Magnitudes of Coupling Constants ¹ C and ¹³ C. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2009, 635, 1087-1091. | 0.6 | 31 |
| 4055 | Ligand Exchange Processes on Solvated Zinc Cations $\hat{\alpha}$ DFT Analysis of Hydrogen Cyanide Exchange on [Zn(HCN) ₆] ²⁺ . Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2009, 635, 1536-1540. | 0.6 | 7 |
| 4056 | The magnetization of $\hat{\alpha}$ Fe ₄ N: theory vs. experiment. Physica Status Solidi (B): Basic Research, 2009, 246, 909-928. | 0.7 | 79 |
| 4057 | Chlorination of ammonia and aliphatic amines by Cl ₂ : DFT study of medium and substituent effects. Journal of Physical Organic Chemistry, 2009, 22, 59-68. | 0.9 | 10 |
| 4058 | Novel pyridyl $\hat{\alpha}$ substituted coumarin and its perchlorate salt $\hat{\alpha}$ crystal structure and spectroscopic properties. Journal of Physical Organic Chemistry, 2009, 22, 726-734. | 0.9 | 1 |
| 4059 | A computational study of stereospecificity in the thermal elimination reaction of menthyl benzoate in the gas phase. Journal of Physical Organic Chemistry, 2009, 22, 971-977. | 0.9 | 142 |
| 4060 | Influence of substitution of oxygen by sulfur on maltol properties. Journal of Physical Organic Chemistry, 2009, 22, 994-1002. | 0.9 | 6 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4061 | Heterocyclic analogs of phenol as novel potential antioxidants. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 1038-1047. | 0.9 | 7 |
| 4062 | Conclusive evidence on the insensitivity of additive rules to the combinational details of exchange and correlation functional in hybrid DFT methods. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 160-170. | 1.0 | 2 |
| 4063 | Stability, spectroscopic constants, and dissociation of CO ²⁺ : A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 469-476. | 1.0 | 4 |
| 4064 | Development of eclipsed and staggered forms in some hydrogen bonded complexes. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 629-638. | 1.0 | 1 |
| 4065 | On the use of the exact exchange optimized effective potential method for static response properties. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3246-3258. | 1.0 | 7 |
| 4066 | Hybrid density functional calculations of nuclear magnetic shieldings using Slater-type orbitals and the zeroth-order regular approximation. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1676-1683. | 1.0 | 74 |
| 4067 | Implementation and benchmark tests of the DFTB method and its application in the ONIOM method. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1841-1854. | 1.0 | 58 |
| 4068 | Intramolecular charge-transfer excitation energies from range-separated hybrid functionals using the Yukawa potential. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1905-1914. | 1.0 | 31 |
| 4069 | Locally range-separated hybrids as linear combinations of range-separated local hybrids. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2023-2032. | 1.0 | 28 |
| 4070 | The chemiionization reactions Ce + O and Ce + O ₂ : Assignment of the observed chemielectron bands. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2068-2079. | 1.0 | 21 |
| 4071 | Relativistic adiabatic time-dependent density functional theory using hybrid functionals and noncollinear spin magnetization. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2091-2112. | 1.0 | 87 |
| 4072 | An <i>ab initio</i> analysis of charge redistribution upon isomerization of retinal in rhodopsin and bacteriorhodopsin. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3131-3141. | 1.0 | 0 |
| 4073 | Ab initio and DFT study of ³¹ P NMR chemical shifts of sphingomyelin and dihydrosphingomyelin lipid molecule. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3685-3693. | 1.0 | 10 |
| 4074 | Weak intra- and intermolecular interactions in a binaphthol imine: an experimental charge-density study on (±)-8-benzhydrylideneamino-1,1'-binaphthyl-2-ol. <i>Acta Crystallographica Section B: Structural Science</i> , 2009, 65, 757-769. | 1.8 | 31 |
| 4075 | Quantum mechanical calculation of aqueous uranium complexes: carbonate, phosphate, organic and biomolecular species. <i>Chemistry Central Journal</i> , 2009, 3, 10. | 2.6 | 64 |
| 4076 | A potential energy surface bifurcation in terpene biosynthesis. <i>Nature Chemistry</i> , 2009, 1, 384-389. | 6.6 | 109 |
| 4077 | Catalytic peroxide oxidation: The structure of key intermediates in the V/H ₂ O ₂ system according to quantum chemical data. <i>Kinetics and Catalysis</i> , 2009, 50, 656-665. | 0.3 | 3 |
| 4078 | Conformational analysis and vibrational spectroscopic investigation of 3-phenylpropylamine. <i>Vibrational Spectroscopy</i> , 2009, 50, 277-284. | 1.2 | 15 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4079 | Conformational investigation of β , γ -dehydropeptides. IX. <i>N</i> -acetyl- β , γ -dehydrobutyryne methylamide: stereoelectronic properties from infrared and theoretical studies*. <i>Chemical Biology and Drug Design</i> , 1998, 52, 72-79. | 1.2 | 13 |
| 4080 | Structural Characterization of a Zinc High-affinity Binding Site in Rhodopsin. <i>Photochemistry and Photobiology</i> , 2009, 85, 479-484. | 1.3 | 11 |
| 4081 | Amination of aryl chlorides and fluorides toward the synthesis of aromatic amines by palladium-catalyzed route or transition metal free way: Scopes and limitations. <i>Journal of Molecular Catalysis A</i> , 2009, 303, 15-22. | 4.8 | 18 |
| 4082 | Relationship between molecular structure and Raman spectra of quinolines. <i>Journal of Molecular Structure</i> , 2009, 924-926, 301-308. | 1.8 | 42 |
| 4083 | Infrared and Raman spectrum, molecular structure and theoretical calculation of 3,4-dichlorophenylboronic acid. <i>Journal of Molecular Structure</i> , 2009, 921, 178-187. | 1.8 | 43 |
| 4084 | The structure elucidation of a new bromophenol metabolite from <i>Polysiphonia urceolata</i> by experimental and DFT theoretical methods. <i>Journal of Molecular Structure</i> , 2009, 929, 1-5. | 1.8 | 9 |
| 4085 | Intrinsic reactivity of uric acid with dioxygen: Towards the elucidation of the catalytic mechanism of urate oxidase. <i>Bioorganic Chemistry</i> , 2009, 37, 111-125. | 2.0 | 12 |
| 4086 | 4-Component relativistic calculation of the magnetically induced current density in the group 15 heteroaromatic compounds. <i>Chemical Physics</i> , 2009, 356, 187-194. | 0.9 | 49 |
| 4087 | An evaluation of exchange-correlation functionals for the calculations of the ionization energies for atoms and molecules. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2009, 171, 18-23. | 0.8 | 21 |
| 4088 | Synthesis, characterization, and cytotoxicity of trimethylplatinum(IV) complexes with 2-thiocytosine and 1-methyl-2-thiocytosine ligands. <i>Inorganica Chimica Acta</i> , 2009, 362, 189-195. | 1.2 | 31 |
| 4089 | Stereochemistry of the reaction products of the oxidative addition reaction of methyl iodide to $[\text{Rh}(\text{C}_4\text{H}_3\text{S})\text{COCHCOR}(\text{CO})(\text{PPh}_3)]$: A NMR and computational study. <i>Inorganica Chimica Acta</i> , 2009, 362, 519-530. | 1.2 | 42 |
| 4090 | Effect of solvent environment on the CO band position in the infrared spectrum of $\text{trans-}[\text{Fe}(\text{CN})_4(\text{CO})_2]^{2-}$. <i>Inorganica Chimica Acta</i> , 2009, 362, 2728-2734. | 1.2 | 3 |
| 4091 | Chiral-at-metal tetrahydrosalen complexes of resolved titanium(IV) <i>sec</i> -butoxides: Ligand wrapping and multiple asymmetric catalytic induction. <i>Inorganica Chimica Acta</i> , 2009, 362, 3134-3146. | 1.2 | 9 |
| 4092 | 3-Alkylsulfanyl-2-arylazo-3-(pyrrolidin-1-yl)-acrylonitriles as masked 1,3-dipoles. <i>Tetrahedron</i> , 2009, 65, 7662-7672. | 1.0 | 17 |
| 4093 | Reaction of Moore's ketene (tert-butylcyanoketene) with 1,3-cyclopentadiene and 1,3-cyclohexadiene. Is periselectivity controlled by the dynamic of trajectories at the bifurcation point?. <i>Tetrahedron</i> , 2009, 65, 7504-7509. | 1.0 | 8 |
| 4094 | From glycerol to chlorohydrin esters using a solvent-free system. Microwave irradiation versus conventional heating. <i>Tetrahedron</i> , 2009, 65, 10370-10376. | 1.0 | 17 |
| 4095 | Synthesis of aryliminoacetonitriles under FVT conditions or by dehydrogenation of arylaminoacetonitriles: an NMR and UV-photoelectron spectroscopy study. <i>Tetrahedron</i> , 2009, 65, 10581-10589. | 1.0 | 15 |
| 4096 | Conformational study of (R)-(+)-limonene in the liquid phase using vibrational spectroscopy (IR, Tj ETQq1 1 0.784314 rgBT /Overlock | 1.8 | 47 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4097 | An ab initio study of the first stage of catalysis in the monomeric aspartic proteinases. Computational and Theoretical Chemistry, 2009, 900, 1-8. | 1.5 | 4 |
| 4098 | Marked variations of proton release energy of the $G\hat{a}^{+}M^{+}$ (M=Li, Na) in the water circumstance. Computational and Theoretical Chemistry, 2009, 900, 9-18. | 1.5 | 0 |
| 4099 | On the performance of the hybrid TPSS meta-GGA functional to study the singlet open-shell structures: A combined theoretical and experimental investigations of the Ni ₂ O ₂ molecule. Computational and Theoretical Chemistry, 2009, 903, 4-10. | 1.5 | 11 |
| 4100 | Low-spin complexes of Ni ²⁺ with six NH ₃ and H ₂ O ligands: A DFT \hat{a} RX3LYP study. Computational and Theoretical Chemistry, 2009, 902, 21-32. | 1.5 | 9 |
| 4101 | Understanding the influence of Lewis acids in the regioselectivity of the Diels \hat{a} Alder reactions of 2-methoxy-5-methyl-1,4-benzoquinone: A DFT study. Computational and Theoretical Chemistry, 2009, 902, 103-108. | 1.5 | 10 |
| 4102 | Ab initio studies of BN-acenes and cyclo BN-acenes electronic properties and their dependence on the molecular size and the number of electrons. Computational and Theoretical Chemistry, 2009, 905, 1-7. | 1.5 | 2 |
| 4103 | Illustration of a TDDFT spatial overlap diagnostic by basis function exponent scaling. Computational and Theoretical Chemistry, 2009, 914, 110-114. | 1.5 | 38 |
| 4104 | Linear regression analysis of molecular energy properties for poly heterocyclic compounds. Computational and Theoretical Chemistry, 2009, 906, 35-40. | 1.5 | 1 |
| 4105 | Geometry and thermodynamic stabilities of rhodanine tautomers and rotamers: Quantum chemical study. Computational and Theoretical Chemistry, 2009, 907, 66-73. | 1.5 | 15 |
| 4106 | On the dependence of electronic properties on geometric structure for cubane derivatives and oligomers with donor and acceptor groups. Computational and Theoretical Chemistry, 2009, 909, 116-121. | 1.5 | 2 |
| 4107 | Partial charges as reactivity descriptors for nitrido complexes. Computational and Theoretical Chemistry, 2009, 913, 1-7. | 1.5 | 15 |
| 4108 | DFT RX3LYP and RPBEPBE studies on the structural, electronic, and vibrational properties of some amino-alcohol ligands. Computational and Theoretical Chemistry, 2009, 915, 20-32. | 1.5 | 12 |
| 4109 | Computational study of adsorption, diffusion, and dissociation of precursor species on the GaN (0001) surface during GaN MOCVD. Surface Science, 2009, 603, L31-L34. | 0.8 | 14 |
| 4110 | On the localization of electron states near silver ion adsorbed on atomic-rough surface of AgCl nanocrystal. Surface Science, 2009, 603, 2564-2573. | 0.8 | 5 |
| 4111 | \hat{a} -1-N-succinimidato complexes of iron, molybdenum and tungsten as reversible inhibitors of papain. Journal of Inorganic Biochemistry, 2009, 103, 1162-1168. | 1.5 | 7 |
| 4112 | Glyphosate complexation to aluminium(III). An equilibrium and structural study in solution using potentiometry, multinuclear NMR, ATR \hat{a} FTIR, ESI-MS and DFT calculations. Journal of Inorganic Biochemistry, 2009, 103, 1426-1438. | 1.5 | 27 |
| 4113 | Electronic properties of defects in polycrystalline dielectric materials. Microelectronic Engineering, 2009, 86, 1751-1755. | 1.1 | 25 |
| 4114 | Effect of a structural modification of the bipyridinium core on the phase behaviour of viologen-based bistriflimide salts. Journal of Molecular Liquids, 2009, 145, 41-47. | 2.3 | 36 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4115 | Determination of the absolute configuration of two estrogenic nonylphenols in solution by chiroptical methods. <i>Journal of Molecular Structure</i> , 2009, 918, 14-18. | 1.8 | 6 |
| 4116 | A novel supramolecular compound of cadmium(II): Synthesis, characterization, crystal structure, ab initio HF, DFT calculations and solution study. <i>Journal of Molecular Structure</i> , 2009, 919, 381-388. | 1.8 | 33 |
| 4117 | Synthesis and anti-leukemia activity mensuration of 1-phenethyl-4-hydroxy-4-substituted piperidinium hydrochlorides: Structure of bis[1-phenethyl-4-hydroxy-4-(3-fluorophenyl) piperidinium hydrochloride] studied by X-ray and DFT methods. <i>Journal of Molecular Structure</i> , 2009, 929, 97-104. | 1.8 | 5 |
| 4118 | Experimental and theoretical studies of the triphenyltin(IV) chloride adduct of pyridine-2-ethanol. <i>Journal of Molecular Structure</i> , 2009, 937, 44-49. | 1.8 | 6 |
| 4119 | Synthesis, structural and conformational study of chromane derivatives. <i>Journal of Molecular Structure</i> , 2009, 937, 139-145. | 1.8 | 5 |
| 4120 | A mechanistic study of the electron capture dissociation of oligonucleotides. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 213-226. | 1.2 | 13 |
| 4121 | Host-guest hydrogen atom transfer induced by electron capture. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 639-651. | 1.2 | 7 |
| 4122 | A new copper containing MALDI matrix that yields high abundances of [Peptide + Cu] ⁺ ions. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 1263-1271. | 1.2 | 14 |
| 4123 | Interaction of the cesium cation with mono-, di-, and tricarboxylic acids in the gas phase. A Cs ⁺ affinity scale for cesium carboxylates ion pairs. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 1912-1924. | 1.2 | 15 |
| 4124 | Structural and magnetic properties of metal complexes with pyridine-2,6-dicarboxylate and 5-(4-bromophenyl)-2,4-bipyridine. <i>Polyhedron</i> , 2009, 28, 980-986. | 1.0 | 9 |
| 4125 | A new χ -acidity scale for several N-donor heterocycles as ligands in neutral gold(III) complexes. <i>Polyhedron</i> , 2009, 28, 1079-1084. | 1.0 | 10 |
| 4126 | Synthesis, structures and in vitro cytotoxicity studies of platinum(IV) complexes with N,S and S,S heterocyclic ligands. <i>Polyhedron</i> , 2009, 28, 3699-3706. | 1.0 | 14 |
| 4127 | Theoretical investigation on the white-light emission from a single-polymer system with simultaneous blue and orange emission. <i>Polymer</i> , 2009, 50, 6172-6185. | 1.8 | 18 |
| 4128 | Ethylene addition to Ru(CH ₂)(O) ₃ π -A theoretical study. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 1081-1090. | 0.8 | 5 |
| 4129 | Four-coordinate boron compounds derived from 2-(2-pyridyl)phenol ligand as novel hole-blocking materials for phosphorescent OLEDs. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 1922-1928. | 0.8 | 34 |
| 4130 | Anticancer drugs based on alkenyl and boryl substituted titanocene complexes. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 1981-1987. | 0.8 | 23 |
| 4131 | Relation between coordination geometry and stereoelectronic properties in DFT models of the CO-inhibited [FeFe]-hydrogenase cofactor. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 2846-2853. | 0.8 | 6 |
| 4132 | Theoretical investigation on possible mechanisms on regioselective formation of (η -3-siloxyallyl)tungsten complexes. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 3456-3461. | 0.8 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4133 | Platina- \hat{I}^2 -diketones as catalysts for hydrosilylation and their reactivity towards hydrosilanes. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 3548-3558. | 0.8 | 30 |
| 4134 | Comparative theoretical study of [3+2] and [2+2] cycloadditions of ethylene and $WXYMe_2$; X, Y=(O), (NH), (CH ₂). <i>Journal of Organometallic Chemistry</i> , 2009, 694, 4090-4093. | 0.8 | 9 |
| 4135 | Triplet excited state characters and photosensitization mechanisms of \hat{I}^{\pm} -terthienyl: A theoretical study. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2009, 94, 51-53. | 1.7 | 9 |
| 4136 | Photochemical and photophysical properties, and photodegradation mechanism, of the non-steroid anti-inflammatory drug Flurbiprofen. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2009, 202, 48-56. | 2.0 | 14 |
| 4137 | Density functional theory study of possible mechanisms of folic acid photodecomposition. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2009, 208, 1-6. | 2.0 | 16 |
| 4138 | Spin-forbidden transitions in flavone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009, 73, 1-5. | 2.0 | 12 |
| 4139 | Vibrational spectra of cysteine zwitterion and mechanism of its formation: Bulk and specific solvent effects and geometry optimization in aqueous media. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009, 73, 719-729. | 2.0 | 22 |
| 4140 | Low-frequency vibrational modes of dl-homocysteic acid and related compounds. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009, 73, 884-891. | 2.0 | 27 |
| 4141 | Quantum chemical studies of molecules incorporating a $Cu_2O_2^{2+}$ core. <i>Coordination Chemistry Reviews</i> , 2009, 253, 723-753. | 9.5 | 90 |
| 4142 | Prediction of molecular properties and molecular spectroscopy with density functional theory: From fundamental theory to exchange-coupling. <i>Coordination Chemistry Reviews</i> , 2009, 253, 526-563. | 9.5 | 927 |
| 4143 | Photoinduced electron transfer from a terrylene dye to TiO_2 : Quantification of band edge shift effects. <i>Chemical Physics</i> , 2009, 357, 124-131. | 0.9 | 19 |
| 4144 | The DFT study on $C\hat{a}^{\epsilon}H$ activation of ethene by YNH^+ and $YC_2H_3N^+$ in gas phase. <i>Chemical Physics</i> , 2009, 363, 1-6. | 0.9 | 5 |
| 4145 | Role of the reacting free radicals on the antioxidant mechanism of curcumin. <i>Chemical Physics</i> , 2009, 363, 13-23. | 0.9 | 104 |
| 4146 | Ab initio molecular simulations with numeric atom-centered orbitals. <i>Computer Physics Communications</i> , 2009, 180, 2175-2196. | 3.0 | 2,170 |
| 4147 | The role of accurate quantum mechanical computations in the assignment of vibrational spectra for unstable free radicals: H_2CN and F_2CN as test cases. <i>Chemical Physics Letters</i> , 2009, 467, 276-280. | 1.2 | 17 |
| 4148 | The reaction mechanism of phenylethanolamine N-methyltransferase: A density functional theory study. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2009, 1794, 1831-1837. | 1.1 | 24 |
| 4149 | DFT study of molybdena \hat{a}^{ϵ} silica system \hat{a}^{ϵ} A selection of density functionals based on their performance in thermochemistry of molybdenum compounds. <i>Chemical Physics Letters</i> , 2009, 469, 140-144. | 1.2 | 30 |
| 4150 | Photoexcitation of 11-Z-cis-7,8-dihydro retinal and 11-Z-cis retinal: A comparative computational study. <i>Chemical Physics Letters</i> , 2009, 469, 224-228. | 1.2 | 20 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 4151 | Binding of Xâ€“H to the lone-pair vacancy: Charge-inverted hydrogen bond. <i>Chemical Physics Letters</i> , 2009, 477, 374-376. | 1.2 | 41 |
| 4152 | Theoretical study of the structure, energetics and vibrational frequencies of waterâ€“acetone and waterâ€“2-butanone complexes. <i>Chemical Physics Letters</i> , 2009, 480, 178-184. | 1.2 | 8 |
| 4153 | Unusual electron density topology and intramolecular steric ï€“ï€“ interaction in 1,3,5,7-cyclooctatetraene. <i>Chemical Physics Letters</i> , 2009, 481, 34-38. | 1.2 | 10 |
| 4154 | Molecular model of CENS piperidine ï²-CD inclusion complex: DFT study. <i>Comptes Rendus Chimie</i> , 2009, 12, 1305-1312. | 0.2 | 24 |
| 4155 | Novel trans-dichloridoplatinum(II) complexes with 3- and 4-acetylpyridine: Synthesis, characterization, DFT calculations and cytotoxicity. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 1921-1925. | 2.6 | 24 |
| 4156 | Novel CYP17 inhibitors: Synthesis, biological evaluation, structureâ€“activity relationships and modelling of methoxy- and hydroxy-substituted methyleneimidazolyl biphenyls. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 2765-2775. | 2.6 | 63 |
| 4157 | Synchrotron radiation VUV double photoionization of CHF ₂ Cl. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2009, 173, 24-28. | 0.8 | 9 |
| 4158 | Synthesis and characterization of a homoleptic titanium dihydrobis(pyrazol-1-yl)borate complex. <i>Inorganic Chemistry Communication</i> , 2009, 12, 1001-1003. | 1.8 | 3 |
| 4159 | Glucose-based spiro-isoxazolines: A new family of potent glycogen phosphorylase inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 7368-7380. | 1.4 | 59 |
| 4160 | QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 395502. | 0.7 | 18,183 |
| 4161 | Theoretical Study of Structure and Electronic Absorption Spectra of Some Schiff Bases and Their Zinc Complexes. <i>Inorganic Chemistry</i> , 2009, 48, 11123-11130. | 1.9 | 56 |
| 4162 | Extensive TD-DFT Benchmark: Singlet-Excited States of Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2420-2435. | 2.3 | 942 |
| 4163 | Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. <i>Journal of Physical Chemistry B</i> , 2009, 113, 6378-6396. | 1.2 | 12,475 |
| 4164 | An Assessment of Theoretical Methods for Nonbonded Interactions: Comparison to Complete Basis Set Limit Coupled-Cluster Potential Energy Curves for the Benzene Dimer, the Methane Dimer, Benzeneâ€“Methane, and Benzeneâ€“H ₂ . <i>Journal of Physical Chemistry A</i> , 2009, 113, 10146-10159. | 1.1 | 369 |
| 4165 | Ring Strain Energy in the Cyclooctyl System. The Effect of Strain Energy on [3 + 2] Cycloaddition Reactions with Azides. <i>Journal of the American Chemical Society</i> , 2009, 131, 5233-5243. | 6.6 | 96 |
| 4166 | 2-Iodoxybenzenesulfonic Acid as an Extremely Active Catalyst for the Selective Oxidation of Alcohols to Aldehydes, Ketones, Carboxylic Acids, and Enones with Oxone. <i>Journal of the American Chemical Society</i> , 2009, 131, 251-262. | 6.6 | 281 |
| 4167 | â€“Mindlessâ€“DFT Benchmarking. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 993-1003. | 2.3 | 215 |
| 4168 | ¹³ C NMR Spectroscopy of â€“Arduengo-typeâ€“Carbenes and Their Derivatives. <i>Chemical Reviews</i> , 2009, 109, 3385-3407. | 23.0 | 308 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4169 | Diels–Alder Reaction between Cyclopentadiene and C ₆₀ : An Analysis of the Performance of the ONIOM Method for the Study of Chemical Reactivity in Fullerenes and Nanotubes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9721-9726. | 1.1 | 63 |
| 4170 | Performance of DFT Methods in the Calculation of Optical Spectra of TCF-Chromophores. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2835-2846. | 2.3 | 54 |
| 4171 | A DFT Study on the Reaction Pathways for Carbon–Carbon Bond-Forming Reactions between Propargylic Alcohols and Alkenes or Ketones Catalyzed by Thiolate-Bridged Diruthenium Complexes. <i>Chemistry - an Asian Journal</i> , 2009, 4, 81-88. | 1.7 | 34 |
| 4172 | On the Effect of Tether Composition on <i>cis</i> / <i>trans</i> Selectivity in Intramolecular Diels–Alder Reactions. <i>Chemistry - an Asian Journal</i> , 2009, 4, 126-134. | 1.7 | 12 |
| 4173 | Mechanistic Investigation of Iron-Catalyzed Coupling Reactions. <i>ChemCatChem</i> , 2009, 1, 152-161. | 1.8 | 119 |
| 4174 | Theory of tunneling across hydrogen-bonded base pairs for DNA recognition and sequencing. <i>Physical Review E</i> , 2009, 79, 051911. | 0.8 | 15 |
| 4175 | Computation of accurate excitation energies for large organic molecules with double-hybrid density functionals. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4611. | 1.3 | 252 |
| 4176 | Kinetic and Thermodynamic Stability of the Group 13 Trihydrides. <i>Inorganic Chemistry</i> , 2009, 48, 7953-7961. | 1.9 | 20 |
| 4177 | Tautomeric forms study of 1H-(2-pyridyl)-3-methyl-5-hydroxypyrazole and 1H-(2-pyridyl)-3-phenyl-5-hydroxypyrazole. Synthesis, structure, and cytotoxic activity of their complexes with palladium(II) ions. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2009, 24, 1257-1268. | 2.5 | 11 |
| 4178 | Octahedral HSiCl ₃ and HSiCl ₂ Me Adducts with Pyridines. <i>Journal of the American Chemical Society</i> , 2009, 131, 6855-6864. | 6.6 | 55 |
| 4179 | On the nature of the chemical bond in heterobimetallic palladium(II) complexes with divalent 3d metals. <i>Russian Journal of Inorganic Chemistry</i> , 2009, 54, 885-892. | 0.3 | 16 |
| 4180 | The thermodynamic characteristics of formation of organic molecule complexes with the magnesium ion in water: The results of quantum-chemical modeling. <i>Russian Journal of Physical Chemistry A</i> , 2009, 83, 565-574. | 0.1 | 1 |
| 4181 | Acyclic Dialkylstannylene and -Plumbylene Compounds That Are Monomeric in the Solid State. <i>Organometallics</i> , 2009, 28, 5661-5668. | 1.1 | 24 |
| 4182 | Application of Multipolar Charge Models and Molecular Dynamics Simulations to Study Stark Shifts in Inhomogeneous Electric Fields. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13199-13209. | 1.1 | 22 |
| 4183 | Single-layered chrysotile nanotubes: A quantum mechanical <i>ab initio</i> simulation. <i>Journal of Chemical Physics</i> , 2009, 131, 204701. | 1.2 | 26 |
| 4184 | Why Is the Suzuki–Miyaura Cross-Coupling of sp ³ Carbons in β -Bromo Sulfoxide Systems Fast and Stereoselective? A DFT Study on the Mechanism. <i>Journal of Organic Chemistry</i> , 2009, 74, 4049-4054. | 1.7 | 54 |
| 4185 | Activation of Carbon–Hydrogen and Hydrogen–Hydrogen Bonds by Copper–Nitrenes: A Comparison of Density Functional Theory with Single- and Multireference Correlation Consistent Composite Approaches. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2959-2966. | 2.3 | 31 |
| 4186 | Dioxapyrene-Based Organic Semiconductors for Organic Field Effect Transistors. <i>Journal of Physical Chemistry C</i> , 2009, 113, 14482-14486. | 1.5 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4187 | Dissociative Adsorption of PH ₃ on the Si(111)-7 × 7 Surface: A Theoretical Investigation. <i>Journal of Physical Chemistry C</i> , 2009, 113, 7843-7850. | 1.5 | 4 |
| 4188 | Solvent Dependence of ¹⁴ N Nuclear Magnetic Resonance Chemical Shielding Constants as a Test of the Accuracy of the Computed Polarization of Solute Electron Densities by the Solvent. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2284-2300. | 2.3 | 9 |
| 4189 | Aspects of the Proton Transfer in Liquid Phosphonic Acid. <i>Journal of Physical Chemistry B</i> , 2009, 113, 8475-8480. | 1.2 | 15 |
| 4190 | Activation of P ₄ by Singlet Silylene (SiH ₂): A Computational Study. <i>Organometallics</i> , 2009, 28, 1289-1294. | 1.1 | 17 |
| 4191 | η ⁵ -Metallocenylmethyl cations and Their Isoelectronic Congeners: A Comparison Based on DFT Calculations. <i>Organometallics</i> , 2009, 28, 1014-1017. | 1.1 | 27 |
| 4192 | Equation of state of hexagonal closed packed iron under Earth's core conditions from quantum Monte Carlo calculations. <i>Physical Review B</i> , 2009, 79, . | 1.1 | 28 |
| 4193 | Terpenylic Acid and Related Compounds from the Oxidation of η ⁵ -Pinene: Implications for New Particle Formation and Growth above Forests. <i>Environmental Science & Technology</i> , 2009, 43, 6976-6982. | 4.6 | 175 |
| 4194 | Gas Phase Absorption Studies of Photoactive Yellow Protein Chromophore Derivatives. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9442-9449. | 1.1 | 56 |
| 4195 | Simulation of Vibrational Spectra of Large Molecules by Arbitrary Time Propagation. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 200-207. | 2.3 | 8 |
| 4196 | Confined But-2-ene Catalytic Isomerization Inside H-ZSM-5 Models: A DFT Study. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1274-1283. | 2.3 | 15 |
| 4197 | Tetraphenylene Ring Flip Revisited. <i>Journal of Organic Chemistry</i> , 2009, 74, 3609-3611. | 1.7 | 36 |
| 4198 | Energies, Geometries, and Charge Distributions of Zn Molecules, Clusters, and Biocenters from Coupled Cluster, Density Functional, and Neglect of Diatomic Differential Overlap Models. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1254-1265. | 2.3 | 67 |
| 4199 | Density Functional Theory Calculations on Mössbauer Parameters of Nonheme Iron Nitrosyls. <i>Inorganic Chemistry</i> , 2009, 48, 9155-9165. | 1.9 | 60 |
| 4200 | Anharmonic Coupling in Molecular Dynamics Simulations of Ligand Vibrational Relaxation in Bound Carbonmonoxy Myoglobin. <i>Journal of Physical Chemistry B</i> , 2009, 113, 13061-13070. | 1.2 | 15 |
| 4201 | Thermally Activated Superradiance and Intersystem Crossing in the Water-Soluble Chlorophyll Binding Protein. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9948-9957. | 1.2 | 56 |
| 4202 | DFT Study of the Transition States and Products of Methyl Radical Addition to Olefins Coordinated in an Asymmetrical Mode to [Cp ₂ Zr(O ^t Bu)] ⁺ : Predictions of Reversed Regioselectivities Compared to the Noncoordinated Reactions. <i>Organometallics</i> , 2009, 28, 6469-6479. | 1.1 | 4 |
| 4203 | Endohedral Nickel, Palladium, and Platinum Atoms in 10-Vertex Germanium Clusters: Competition between Bicapped Square Antiprismatic and Pentagonal Prismatic Structures. <i>Journal of Physical Chemistry A</i> , 2009, 113, 527-533. | 1.1 | 28 |
| 4204 | Gosteli's Claisen Rearrangement: DFT Study of Substituent Rate Effects. <i>Journal of Organic Chemistry</i> , 2009, 74, 4336-4342. | 1.7 | 30 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4205 | Mechanism of S ₂ H ₂ Reactions of Disulfides: Frontside vs Backside, Stepwise vs Concerted. <i>Journal of Organic Chemistry</i> , 2009, 74, 5356-5360. | 1.7 | 31 |
| 4206 | Energetics and Dynamics of the Reactions of O(3P) with Dimethyl Methylphosphonate and Sarin. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13752-13761. | 1.1 | 7 |
| 4207 | Toward the Photoinduced Reactivity of 1,5-Diphenylpenta-1,4-diyne-3-one (DPD): Real-Time Investigations by Magnetic Resonance. <i>Macromolecules</i> , 2009, 42, 8034-8038. | 2.2 | 21 |
| 4208 | Unexpected Trimerization of Pyrazine in the Coordination Sphere of Low-Valent Titanocene Fragments. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2044-2049. | 2.3 | 12 |
| 4209 | Ligands for Dinitrogen Fixation at Schrock-Type Catalysts. <i>Inorganic Chemistry</i> , 2009, 48, 1638-1648. | 1.9 | 58 |
| 4210 | Evaluation of Density Functionals and Basis Sets for Carbohydrates. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 679-692. | 2.3 | 183 |
| 4211 | Allenyl Azide Cycloaddition Chemistry. 2,3-Cyclopentenediolated Indole Synthesis through Indolidene Intermediates. <i>Journal of Organic Chemistry</i> , 2009, 74, 4958-4974. | 1.7 | 41 |
| 4212 | Water Exchange Mechanism in the First Excited State of Hydrated Uranyl(VI). <i>Inorganic Chemistry</i> , 2009, 48, 11310-11313. | 1.9 | 14 |
| 4213 | The Binding of Ag ⁺ and Au ⁺ to Ethene. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7474-7481. | 1.1 | 28 |
| 4214 | Thermal Rearrangements of 2-Ethynylbiphenyl: A DFT Study of Competing Reaction Mechanisms. <i>Journal of Organic Chemistry</i> , 2009, 74, 499-503. | 1.7 | 29 |
| 4215 | Cyclopolymerization Reactions of Diallyl Monomers: Exploring Electronic and Steric Effects Using DFT Reactivity Indices. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8704-8711. | 1.1 | 32 |
| 4216 | Combined Crossed Molecular Beam and Theoretical Studies of the N ₂ D + CH ₄ Reaction and Implications for Atmospheric Models of Titan. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11138-11152. | 1.1 | 90 |
| 4217 | Aqueous Coordination Chemistry of H ₂ : Why is Coordinated H ₂ Inert to Substitution by Water in <i>trans</i> -Ru(P ₂) ₂ (H ₂)H ⁺ -type Complexes (P ₂ = a Chelating Phosphine)? <i>Inorganic Chemistry</i> , 2009, 48, 2976-2984. | 1.9 | 11 |
| 4218 | Vibrationally Induced Interconversion of H-Bonded NO ₂ ⁺ ·H ₂ O Isomers within NO ₂ ⁺ ·H ₂ O·Ar _m Clusters Using IR Pump-Probe through the OH and NO Stretching Vibrations. <i>Journal of Physical Chemistry A</i> , 2009, 113, 975-981. | 1.1 | 15 |
| 4219 | Theoretical Investigations on Mechanisms of Pd(OAc) ₂ -Catalyzed Intramolecular Diaminations in the Presence of Bases and Oxidants. <i>Organometallics</i> , 2009, 28, 4507-4512. | 1.1 | 34 |
| 4220 | DFT-Based Explanation of the Effect of Simple Anionic Ligands on the Regioselectivity of the Heck Arylation of Acrolein Acetals. <i>Organometallics</i> , 2009, 28, 6201-6205. | 1.1 | 23 |
| 4221 | Expanding the Coordination Cage: A Ruthenium(II) Polypyridine Complex Exhibiting High Quantum Yields under Ambient Conditions. <i>Inorganic Chemistry</i> , 2009, 48, 5677-5684. | 1.9 | 73 |
| 4222 | Searching for Microporous, Strongly Basic Catalysts: Experimental and Calculated ²⁹ Si NMR Spectra of Heavily Nitrogen-Doped Y Zeolites. <i>Journal of the American Chemical Society</i> , 2009, 131, 11062-11079. | 6.6 | 47 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4223 | Performance of Ab Initio and Density Functional Methods for Conformational Equilibria of C_nH_{2n+2} Alkane Isomers ($n = 4\text{--}8$). <i>Journal of Physical Chemistry A</i> , 2009, 113, 11974-11983. | 1.1 | 156 |
| 4224 | Hydrogenated Monolayer Sheets of Group 13 [–] 15 Binary Compounds: Structural and Electronic Characteristics. <i>Journal of Physical Chemistry C</i> , 2009, 113, 229-234. | 1.5 | 16 |
| 4225 | Spin Crossover-Coupled Electron Transfer of $[M(\text{tacn})_2]^{3+/2+}$ Complexes (tacn =) $1,4,7\text{-T}$ $6189\text{--}6197$. | 6.6 | 41 |
| 4226 | Quantitative Assessment of Electrostatic Embedding in Density Functional Theory Calculations of Biomolecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2257-2264. | 2.3 | 6 |
| 4227 | High-Resolution and Dispersed Fluorescence Examination of Vibronic Bands of Tryptamine: Spectroscopic Signatures for L_a/L_b Mixing near a Conical Intersection. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2456-2466. | 1.1 | 28 |
| 4228 | Twisting the Phenyls in Aryl Diphosphenes ($Ar^*P^*P^*Ar$). Significant Impact upon Lowest Energy Excited States. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7054-7063. | 1.1 | 31 |
| 4229 | Mechanism of the Ni(0)-Catalyzed Vinylcyclopropane \rightarrow Cyclopentene Rearrangement. <i>Journal of Organic Chemistry</i> , 2009, 74, 7822-7833. | 1.7 | 59 |
| 4230 | Electron Super-Rich Radicals. III. On the Peculiar Behavior of the Aminodihydroxymethyl Radical in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5855-5864. | 1.1 | 5 |
| 4231 | The Unique Palladium-Centered Pentagonal Antiprismatic Cationic Bismuth Cluster: A Comparison of Related Metal-Centered 10-Vertex Pnictogen Cluster Structures by Density Functional Theory. <i>Inorganic Chemistry</i> , 2009, 48, 8508-8514. | 1.9 | 19 |
| 4232 | Infrared spectra, structure and bonding in the LiO_2 , LiO_2Li , LiO and Li_2O molecules in solid neon. <i>Molecular Physics</i> , 2009, 107, 739-748. | 0.8 | 49 |
| 4233 | Local Hybrid Functionals with an Explicit Dependence on Spin Polarization. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11898-11906. | 1.1 | 43 |
| 4234 | Efficient Diffuse Basis Sets: cc-pV xZ and maug-cc-pV xZ . <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1197-1202. | 2.3 | 236 |
| 4235 | Block-Localized Density Functional Theory (BLDFT), Diabatic Coupling, and Their Use in Valence Bond Theory for Representing Reactive Potential Energy Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2702-2716. | 2.3 | 110 |
| 4236 | Kinetic C^*H Oxidative Addition vs Thermodynamic C^*X Oxidative Addition of Chlorobenzene by a Neutral Rh(I) System. A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11706-11712. | 1.1 | 13 |
| 4237 | Gas-Phase Thermochemical Properties of the Damaged Base O6-Methylguanine versus Adenine and Guanine. <i>Journal of Organic Chemistry</i> , 2009, 74, 7429-7440. | 1.7 | 44 |
| 4238 | Tunnel Currents across Silane Diamines/Dithiols and Alkane Diamines/Dithiols: A Comparative Computational Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 744-750. | 1.5 | 38 |
| 4239 | Investigation of Reverse-Hydrogen Spillover on Zeolite-Supported Palladium Tetramer by ONIOM Method. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16070-16076. | 1.5 | 15 |
| 4240 | Adsorbed CO on Group 10 Metal Fragments: A DFT Study. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1223-1233. | 2.5 | 6 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4241 | Mechanisms for Formation of Diazocinones, Pyridazines, and Pyrazolines from Tetrazinesâ€”Oxyanion-Accelerated Pericyclic Cascades?. <i>Journal of Organic Chemistry</i> , 2009, 74, 4804-4811. | 1.7 | 18 |
| 4242 | Structural Insights into the Binding of Uranyl with Human Serum Protein Apotransferrin Structure and Spectra of Proteinâ€”Uranyl Interactions. <i>Chemical Research in Toxicology</i> , 2009, 22, 1613-1621. | 1.7 | 28 |
| 4243 | Conformational Study of a Bent-Core Liquid Crystal: ¹³ C NMR and DFT Computation Approach. <i>Journal of Physical Chemistry B</i> , 2009, 113, 14062-14072. | 1.2 | 46 |
| 4244 | Siliconâ€”Bismuth and Germaniumâ€”Bismuth Clusters of High Stability. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12079-12087. | 1.1 | 25 |
| 4245 | Electronic Structure of the Metal Center in the Cd ²⁺ , Zn ²⁺ , and Cu ²⁺ Substituted Forms of KDO8P Synthase: Implications for Catalysis. <i>Biochemistry</i> , 2009, 48, 3610-3630. | 1.2 | 13 |
| 4246 | Role of Dimethyl Sulfoxide in the Hydrolytic Peeling of Boron Nitride Nanotubes. <i>Journal of Physical Chemistry C</i> , 2009, 113, 15565-15568. | 1.5 | 8 |
| 4247 | Theoretical Studies on Structures and Spectroscopic Properties of Cyclometalated Gold(III) Complexes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9396-9403. | 1.1 | 20 |
| 4248 | Perturbations of Membrane Structure by Cholesterol and Cholesterol Derivatives Are Determined by Sterol Orientation. <i>Journal of the American Chemical Society</i> , 2009, 131, 4854-4865. | 6.6 | 77 |
| 4249 | Bonding and Magnetism of Fe ₆ (C ₆ H ₆) ₂ , <i>Journal of Physical Chemistry A</i> , 2009, 113, 6222-6238. | 1.1 | 17 |
| 4250 | Synthesis and Reactivity of Titanium and Zirconium Complexes Supported by a Multidentate Monoanionic [N ₂ P ₂] Ligand. <i>Organometallics</i> , 2009, 28, 3338-3349. | 1.1 | 27 |
| 4251 | First Principles Studies of Fe-Containing Aluminosilicate and Aluminogermanate Nanotubes. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3224-3231. | 2.3 | 19 |
| 4252 | Structural Study of Ga(III), In(III), and Fe(III) Complexes of Triaza-Macrocyclic Based Ligands with N3S3 Donor Set. <i>Inorganic Chemistry</i> , 2009, 48, 3257-3267. | 1.9 | 23 |
| 4253 | Deprotonation Mechanism of New Antihypertensive Piperidinylmethylphenols: A Combined Experimental and Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2009, 113, 11765-11774. | 1.2 | 7 |
| 4254 | A Redox Non-Innocent Ligand Controls the Life Time of a Reactive Quartet Excited State - An MCSCF Study of [Ni(H)(OH)] ⁺ . <i>Journal of the American Chemical Society</i> , 2009, 131, 12634-12642. | 6.6 | 36 |
| 4255 | Theoretical Mechanistic Study of the Oxidative Degradation of Benzene in the Troposphere: Reaction of Benzeneâ€”HO Radical Adduct with O ₂ . <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1607-1623. | 2.3 | 41 |
| 4256 | Structure-Based Rationale for Selectivity in the Asymmetric Allylic Alkylation of Cycloalkenyl Esters Employing the Trost â€”Standard Ligandâ€” (TSL): Isolation, Analysis and Alkylation of the Monomeric form of the Cationic Ir ³⁺ -Cyclohexenyl Complex [(Ir ³⁺ -C ₆ H ₉)Pd(TSL)] ⁺ . <i>Journal of the American Chemical Society</i> , 2009, 131, 8815-8827. | 6.6 | 166 |
| 4257 | Photochemical Reaction of Mo(CO) ₆ with Et ₂ GeH ₂ : NMR and DFT Studies of Reaction Products; Crystal Structure of a Novel Complex [(Mo(Î¼ ₄ -Ir ²⁺ -Hâ€”GeEt ₂)(CO) ₄)] ₂ . <i>Organometallics</i> , 2009, 28, 5857-5865. | 1.1 | 21 |
| 4258 | A Bis(acetyl)-Bridged Platinum(II) Coordination Polymer as a Building Block for Diacetylplatinum(II) Complexes and Platina-Î²-diketones. <i>Organometallics</i> , 2009, 28, 2485-2493. | 1.1 | 14 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4259 | Fully Relativistic, Comparative Investigation of Gold and Platinum Alkyne Complexes of Relevance for the Catalysis of Nucleophilic Additions to Alkynes. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2717-2725. | 2.3 | 192 |
| 4260 | Nature of Low-Lying Excited States in H-Aggregated Perylene Bisimide Dyes: Results of TD-LRC-DFT and the Mixed Exciton Model. <i>Journal of Physical Chemistry B</i> , 2009, 113, 14581-14587. | 1.2 | 33 |
| 4261 | Molecular Orbital-Averaged Fukui Function for the Reactivity Description of Alkaline Earth Metal Oxide Clusters. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1245-1253. | 2.3 | 22 |
| 4262 | Defective to fully coordinated crossover in complex directionally bonded nanoclusters. <i>Physical Review B</i> , 2009, 80, . | 1.1 | 17 |
| 4263 | Structure, Bonding, and Relative Stability of the Ground and Low-Lying Electronic States of CuO ₂ . The Role of Exact Exchange. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1308-1317. | 1.1 | 19 |
| 4264 | Theoretical Study on Rotation of Pyrrole Rings in Porphyrin and N-Confused Porphyrin. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13953-13963. | 1.1 | 37 |
| 4265 | Dynamic Behavior of Intramolecularly Base-Stabilized Phosphatetrylenes. Insights into the Inversion Processes of Trigonal Pyramidal Germanium(II) and Tin(II) Centers. <i>Organometallics</i> , 2009, 28, 3327-3337. | 1.1 | 37 |
| 4266 | Structural Evolution, Sequential Oxidation, and Chemical Bonding in Tritantalum Oxide Clusters: Ta ₃ O _n ⁺ and Ta ₃ O _n (n = 1-8). <i>Journal of Physical Chemistry A</i> , 2009, 113, 9804-9813. | 1.1 | 48 |
| 4267 | Fast Substitution Reactions of Pt(II) in Different Ionic Liquids. Reactivity Control by Anionic Components. <i>Inorganic Chemistry</i> , 2009, 48, 588-597. | 1.9 | 31 |
| 4268 | Mechanism of Helix Induction in Poly(4-carboxyphenyl isocyanide) with Chiral Amines and Memory of the Macromolecular Helicity and Its Helical Structures. <i>Journal of the American Chemical Society</i> , 2009, 131, 10719-10732. | 6.6 | 104 |
| 4269 | Oxidative Addition of Iodomethane to Charge-Tuned Rhodium(I) Complexes. <i>Organometallics</i> , 2009, 28, 2062-2071. | 1.1 | 7 |
| 4270 | First-Principles Thermochemistry for the Combustion of a TiCl ₄ and AlCl ₃ Mixture. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13790-13796. | 1.1 | 23 |
| 4271 | Isocyanide Complexes with Platinum and Palladium and Their Reactivity toward Cycloadditions with Nitrones to Form Aminooxycarbenes: A Theoretical Study. <i>Organometallics</i> , 2009, 28, 6593-6602. | 1.1 | 28 |
| 4272 | Long-Range-Corrected Hybrids Based on a New Model Exchange Hole. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 754-762. | 2.3 | 72 |
| 4273 | Carboxyl-Catalyzed Prototropic Rearrangements in Histidine Peptide Radicals upon Electron Transfer: Effects of Peptide Sequence and Conformation. <i>Journal of the American Chemical Society</i> , 2009, 131, 16472-16487. | 6.6 | 26 |
| 4274 | Electronic Structures of Bis- and Monothiophene Complexes with Fe, Co, Ni: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10291-10298. | 1.1 | 5 |
| 4275 | Theoretical Analysis of Kinetic Isotope Effects on Proton Transfer Reactions between Substituted β -Methoxystyrenes and Substituted Acetic Acids. <i>Journal of the American Chemical Society</i> , 2009, 131, 13963-13971. | 6.6 | 30 |
| 4276 | Potential for C-H Activation in CH ₄ Utilizing a CuMFI-Type Zeolite as a Catalyst. <i>Journal of Physical Chemistry C</i> , 2009, 113, 7213-7222. | 1.5 | 32 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4277 | Tetrakis(thiadiazole)porphyrazines. 6. Spectroelectrochemical and Density Functional Theory Studies of the Anions [TTDPzM] ⁿ⁻ (n = 1-4; M = ZnII, MgII(H ₂ O), CuII, 2HI). <i>Inorganic Chemistry</i> , 2009, 48, 9890-9903. | 1.9 | 17 |
| 4278 | Benchmark Data for Noncovalent Interactions in HCOOH- π -Benzene Complexes and Their Use for Validation of Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2726-2733. | 2.3 | 30 |
| 4279 | Coordination of (Glycyl) _n glycine (n = 1-3) to Co ²⁺ and Co ³⁺ . <i>Journal of Physical Chemistry A</i> , 2009, 113, 8883-8892. | 1.1 | 9 |
| 4280 | From <i>closoclo</i> to <i>isoclosoclo</i> Structures and Beyond in Cobaltaboranes with 9 to 12 Vertices. <i>Inorganic Chemistry</i> , 2009, 48, 10117-10125. | 1.9 | 7 |
| 4281 | Comparative Analysis of IR and Vibrational Circular Dichroism Spectra for a Series of Camphor-Related Molecules. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11390-11405. | 1.1 | 37 |
| 4282 | Synthesis, Structures, and Properties of Mixed Dithiolene-Carbonyl and Dithiolene-Phosphine Complexes of Tungsten. <i>Inorganic Chemistry</i> , 2009, 48, 2103-2113. | 1.9 | 41 |
| 4283 | Nonconventional Behavior of NCN-Chelated Organoantimony(III) Sulfide and Isolation of Cyclic Organoantimony(III) Bis(pentasulfide). <i>Inorganic Chemistry</i> , 2009, 48, 10495-10497. | 1.9 | 35 |
| 4284 | Theoretical Analysis of the Unusual Temperature Dependence of the Kinetic Isotope Effect in Quinol Oxidation. <i>Journal of the American Chemical Society</i> , 2009, 131, 7094-7102. | 6.6 | 40 |
| 4285 | Application of Dispersion-Corrected Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10321-10326. | 1.1 | 35 |
| 4286 | Thermochemical Kinetics for Multireference Systems: Addition Reactions of Ozone. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5786-5799. | 1.1 | 114 |
| 4287 | Computational Study of Cesium Cation Interactions with Neutral and Anionic Compounds Related to Soil Organic Matter. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10734-10744. | 1.1 | 19 |
| 4288 | Extension of the Tryptophan $\chi_{2,1}$ Dihedral Angle- ν_{3} Band Frequency Relationship to a Full Rotation: Correlations and Caveats. <i>Biochemistry</i> , 2009, 48, 2777-2787. | 1.2 | 22 |
| 4289 | H/Br Exchange in BBr ₃ by HSiR ₃ (R = H, CH ₃) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 267 Td (C_s). <i>Journal of Physical Chemistry A</i> , 2009, 113, 12035-12043. | 1.1 | 12 |
| 4290 | Theoretical Study on Reactions of HO ₂ Radical with Photodissociation Products of Cl ₂ SO (ClSO and SO). <i>Journal of Physical Chemistry A</i> , 2009, 113, 9981-9987. | 1.1 | 9 |
| 4291 | Synthesis and Characterization of NaBD ₃ H, A Potential Structural Probe for Hydrogen Storage Materials. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13932-13936. | 1.1 | 9 |
| 4292 | Reductive Half-Reaction of Aldehyde Oxidoreductase toward Acetaldehyde: A Combined QM/MM Study. <i>Journal of the American Chemical Society</i> , 2009, 131, 4628-4640. | 6.6 | 38 |
| 4293 | Cation Environment of BaCeO ₃ -Based Protonic Conductors: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6381-6390. | 1.1 | 11 |
| 4294 | Quantum Chemical Studies on High-Valent Metal Nitrido Derivatives of Keggin-Type Polyoxometalates ([PW ₁₁ O ₃₉ {MVIN}] ₄ ⁻ (M = Ru, Os, Re)): MVI ⁻ N Bonding and Electronic Structures. <i>Inorganic Chemistry</i> , 2009, 48, 541-548. | 1.9 | 40 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4295 | Unified Inter- and Intramolecular Dispersion Correction Formula for Generalized Gradient Approximation Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2950-2958. | 2.3 | 76 |
| 4296 | Density Functional Theory Study of the Manganese-Containing Ribonucleotide Reductase from <i>Chlamydia trachomatis</i> : Why Manganese Is Needed in the Active Complex. <i>Biochemistry</i> , 2009, 48, 1878-1887. | 1.2 | 41 |
| 4297 | Theoretical Survey of the Potential Energy Surface of Ti ⁺ + Methanol Reaction. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7103-7111. | 1.1 | 14 |
| 4298 | Probing the Mechanism of O ₂ Activation by a Copper(I) Biomimetic Complex of a C ^H Hydroxylating Copper Monooxygenase. <i>Inorganic Chemistry</i> , 2009, 48, 4062-4066. | 1.9 | 42 |
| 4299 | O-Abstraction Reactions of Nitrous Oxide with Cp ₂ Ti(II) and Other Middle Transition Metal Complexes. <i>Organometallics</i> , 2009, 28, 1158-1164. | 1.1 | 26 |
| 4300 | Effects of ZSM-5 Zeolite Confinement on Reaction Intermediates during Dioxygen Activation by Enclosed Dicopper Cations. <i>Inorganic Chemistry</i> , 2009, 48, 508-517. | 1.9 | 68 |
| 4301 | Benzenium ⁺ Ethene Complex: A Fundamental Problem for Standard Second-Order M ^{ller} -Plesset Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3005-3008. | 1.1 | 19 |
| 4302 | Effects of Electron-Deficient β^2 -Diketiminato and Formazan Supporting Ligands on Copper(I)-Mediated Dioxygen Activation. <i>Inorganic Chemistry</i> , 2009, 48, 4514-4523. | 1.9 | 69 |
| 4303 | Density Functional Study of the Ground and Excited State Potential Energy Surfaces of a Light-Driven Rotary Molecular Motor (3R ₃)-(P ₂)-trans-1,1 ² ,2,2 ³ ,3,3 ⁴ -Octahydro-3,3 ¹ -dimethyl-4,4 ³³ -biphenanthryl. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11630-11634. | 1.1 | 33 |
| 4304 | DFT Studies on Reactions of Transition Metal Complexes with O ₂ . <i>Organometallics</i> , 2009, 28, 4443-4451. | 1.1 | 25 |
| 4305 | Selective Decomposition of Alkyl Hydroperoxides on H-Type Zeolite via a Concerted Approach. <i>Journal of Physical Chemistry B</i> , 2009, 113, 1418-1422. | 1.2 | 6 |
| 4306 | Influence of Fluorine Atoms and Aromatic Rings on the Acidity of Ethanol. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10753-10758. | 1.1 | 11 |
| 4307 | Optical Absorptions of New Blue-Light Emitting Oligoquinolines Bearing Pyrenyl and Triphenyl Endgroups Investigated with Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 866-872. | 2.3 | 5 |
| 4308 | Structure Prediction of Bis(amino acidato)copper(II) Complexes with a New Force Field for Molecular Modeling. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1940-1954. | 2.3 | 24 |
| 4309 | Reversible Neutral Dissociation of the N ⁺ Si Dative Bond in Hexacoordinate Hydrido Complexes of Silicon. <i>Organometallics</i> , 2009, 28, 512-516. | 1.1 | 16 |
| 4310 | Structural and Electronic Trends among Group 15 Elemental Nanotubes. <i>Journal of Physical Chemistry C</i> , 2009, 113, 12220-12224. | 1.5 | 19 |
| 4311 | Electronic Structure and Spectroscopy of [Ru(tpy) ₂] ²⁺ , [Ru(tpy)(bpy)(H ₂ O)] ²⁺ , and [Ru(tpy)(bpy)(Cl)] ⁺ . <i>Inorganic Chemistry</i> , 2009, 48, 10720-10725. | 1.9 | 91 |
| 4312 | Influence of the LOV Domain on Low-Lying Excited States of Flavin: A Combined Quantum-Mechanics/Molecular-Mechanics Investigation. <i>Journal of Physical Chemistry B</i> , 2009, 113, 15610-15618. | 1.2 | 49 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4313 | Solvation Dynamics and Adsorption on Ag Hydrosols of Oxazole: A Raman and Computational Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 15198-15205. | 1.1 | 16 |
| 4314 | A Density Functional Theory Study of the Topology of the Charge Density of Complexes of 8-Hydroxyquinoline with Mn(III), Fe(III), and Co(III). <i>Journal of Physical Chemistry A</i> , 2009, 113, 5205-5211. | 1.1 | 6 |
| 4315 | Validation of broken-symmetry density functional methods for the calculation of electron paramagnetic resonance parameters of dinuclear mixed-valence Mn ^{IV} Mn ^{III} complexes. <i>Canadian Journal of Chemistry</i> , 2009, 87, 1521-1539. | 0.6 | 39 |
| 4316 | Thermo-chemical and thermo-physical properties of stishovite: An ab-initio all-electron investigation. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009, 33, 457-468. | 0.7 | 27 |
| 4317 | Quantum chemical study of the Fe(III)-desferrioxamine B siderophore complex—Electronic structure, vibrational frequencies, and equilibrium Fe-isotope fractionation. <i>Geochimica Et Cosmochimica Acta</i> , 2009, 73, 1-12. | 1.6 | 67 |
| 4318 | Crocetane: A potential marker of photic zone euxinia in thermally mature sediments and crude oils of Devonian age. <i>Organic Geochemistry</i> , 2009, 40, 1-11. | 0.9 | 45 |
| 4319 | Probing stereoselectivity and pro-chirality of hydride transfer during short-chain alcohol dehydrogenase activity: A combined quantitative 2H NMR and computational approach. <i>Archives of Biochemistry and Biophysics</i> , 2009, 482, 42-51. | 1.4 | 7 |
| 4320 | Ruthenium-Catalyzed Intramolecular Amination Reactions of Aryl- and Vinylazides. <i>Organometallics</i> , 2009, 28, 6847-6854. | 1.1 | 117 |
| 4321 | Substituent effects in mono- and disubstituted 1,3,5,7-cyclooctatetraene derivatives in natural and planar conformations. <i>New Journal of Chemistry</i> , 2009, 33, 1753. | 1.4 | 22 |
| 4322 | Cleavage of Carbon Dioxide by an Iridium-Supported Fischer Carbene. A DFT Investigation. <i>Journal of the American Chemical Society</i> , 2009, 131, 5800-5808. | 6.6 | 43 |
| 4323 | Intramolecular Hydrogen Bond-Controlled Prolyl Amide Isomerization in Glucosyl 3-(S)-Hydroxy-5-hydroxymethylproline Hybrids: Influence of a C-5-Hydroxymethyl Substituent on the Thermodynamics and Kinetics of Prolyl Amide Cis/Trans Isomerization. <i>Journal of Organic Chemistry</i> , 2009, 74, 3735-3743. | 1.7 | 19 |
| 4324 | Vinyl Acetate Synthesis on Homogeneous and Heterogeneous Pd-Based Catalysts: A Theoretical Analysis on the Reaction Mechanisms. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11758-11762. | 1.1 | 13 |
| 4325 | Density functional theory for transition metals and transition metal chemistry. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 10757. | 1.3 | 1,431 |
| 4326 | Magnetic anisotropy from density functional calculations. Comparison of different approaches: Mn12O12 acetate as a test case. <i>Journal of Chemical Physics</i> , 2009, 130, 194109. | 1.2 | 68 |
| 4327 | The calculation of adiabatic-connection curves from full configuration-interaction densities: Two-electron systems. <i>Journal of Chemical Physics</i> , 2009, 130, 104111. | 1.2 | 64 |
| 4328 | Silver-catalysed protodecarboxylation of carboxylic acids. <i>Chemical Communications</i> , 2009, , 7173. | 2.2 | 181 |
| 4329 | Interrelations between the Mesomeric and Electronegativity Effects in <i>Para</i> -Substituted Derivatives of Phenol/Phenolate and Aniline/Anilide H-Bonded Complexes: A DFT-Based Computational Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5800-5805. | 1.1 | 5 |
| 4330 | Predicting Raman Spectra Using Density Functional Theory. <i>Applied Spectroscopy</i> , 2009, 63, 733-741. | 1.2 | 29 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4331 | Spectroscopic Characterization of the SH2- and Active Site-Directed Peptide Sequences of a Bivalent Src Kinase Inhibitor. <i>Applied Spectroscopy</i> , 2009, 63, 767-774. | 1.2 | 4 |
| 4332 | Long-range corrected double-hybrid density functionals. <i>Journal of Chemical Physics</i> , 2009, 131, 174105. | 1.2 | 327 |
| 4333 | Excitation Energies of Zinc Porphyrin in Aqueous Solution Using Long-Range Corrected Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6041-6043. | 1.1 | 60 |
| 4335 | A Combined QM/MM Study on the Reductive Half-Reaction of Xanthine Oxidase: Substrate Orientation and Mechanism. <i>Journal of the American Chemical Society</i> , 2009, 131, 14885-14902. | 6.6 | 70 |
| 4336 | The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 808-821. | 2.3 | 462 |
| 4337 | The quest for alternative routes to racemic and nonracemic azahelicene derivatives. <i>Collection of Czechoslovak Chemical Communications</i> , 2009, 74, 189-215. | 1.0 | 17 |
| 4338 | Tetrahedranes. A theoretical study of singlet $E_{4^4}H_{4^4}$ molecules ($E = \text{Ca}^{\text{--}}\text{Pb}$ and Tj). <i>ETQq0.0.0 rgBT / Overlock 1</i> | 0.8 | 27 |
| 4339 | Spontaneous Self-Assembly of Silica Nanocages into Inorganic Framework Materials. <i>Journal of Physical Chemistry C</i> , 2009, 113, 518-523. | 1.5 | 16 |
| 4340 | Consequences of Conformational Preorganization in Sesquiterpene Biosynthesis: Theoretical Studies on the Formation of the Bisabolene, Curcumene, Acoradiene, Zizaene, Cedrene, Duprezianene, and Sesquithuriferol Sesquiterpenes. <i>Journal of the American Chemical Society</i> , 2009, 131, 7999-8015. | 6.6 | 113 |
| 4341 | Averaging Semiempirical NMR Chemical Shifts: Dynamic Effects on the Subpicosecond Time Scale. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11723-11733. | 1.1 | 6 |
| 4342 | Benzothiopyranoindole-Based Antiproliferative Agents: Synthesis, Cytotoxicity, Nucleic Acids Interaction, and Topoisomerases Inhibition Properties. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 5429-5441. | 2.9 | 30 |
| 4343 | A Multi-standard Approach for GIAO ^{13}C NMR Calculations. <i>Journal of Organic Chemistry</i> , 2009, 74, 7254-7260. | 1.7 | 208 |
| 4344 | Ligand exchange processes on the smallest solvated alkali and alkaline earth metal cations: An experimental and theoretical approach. <i>Advances in Inorganic Chemistry</i> , 2009, 61, 523-571. | 0.4 | 28 |
| 4345 | Turn-On Fluorescence Detection of Cyanide in Water: Activation of Latent Fluorophores through Remote Hydrogen Bonds That Mimic Peptide β -Turn Motif. <i>Journal of the American Chemical Society</i> , 2009, 131, 16283-16291. | 6.6 | 187 |
| 4346 | A Comprehensive Theoretical Study on the Coupling Reaction Mechanism of Propylene Oxide with Carbon Dioxide Catalyzed by Copper(I) Cyanomethyl. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6710-6723. | 1.1 | 45 |
| 4347 | Ground State Structures of $\text{Fe}_2\text{O}_4^{6+}$ Clusters Probed by Reactions with N_2 . <i>Journal of Physical Chemistry A</i> , 2009, 113, 5302-5309. | 1.1 | 47 |
| 4348 | Strong Conductance Variation in Conformationally Constrained Oligosilane Tunnel Junctions. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3876-3880. | 1.1 | 48 |
| 4349 | The Mechanism of the Catalytic Functionalization of Haloalkanes by Carbene Insertion: An Experimental and Theoretical Study. <i>Organometallics</i> , 2009, 28, 5968-5981. | 1.1 | 49 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4350 | Spectral Properties of Spirooxazine Photochromes: TD-DFT Insights. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13004-13012. | 1.1 | 34 |
| 4351 | First-principles semiclassical initial value representation molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 3861. | 1.3 | 70 |
| 4352 | Interplay between Intramolecular Resonance-Assisted Hydrogen Bonding and Local Aromaticity. II. 1,3-Dihydroxyaryl-2-aldehydes. <i>Journal of Organic Chemistry</i> , 2009, 74, 2059-2066. | 1.7 | 68 |
| 4353 | Calculation of the lattice constant of solids with semilocal functionals. <i>Physical Review B</i> , 2009, 79, . | 1.1 | 709 |
| 4354 | Thermochemistry of Bithiophenes and Thienyl Radicals. A Calorimetric and Computational Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11042-11050. | 1.1 | 25 |
| 4355 | Observed enhancement of the reactivity of a biomimetic diiron complex by the addition of water - mechanistic insights from theoretical modeling. <i>Dalton Transactions</i> , 2009, , 6741. | 1.6 | 18 |
| 4356 | Au(I)-Catalyzed Cycloisomerization Reaction of Amide- or Ester-Tethered 1,6-Enynes to Bicyclo[3.2.0]hept-6-en-2-ones. <i>Journal of Organic Chemistry</i> , 2009, 74, 7922-7934. | 1.7 | 68 |
| 4357 | Paramagnetic Perturbation of the ¹⁹ F NMR Chemical Shift in Fluorinated Cysteine by O ₂ : A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10916-10922. | 1.2 | 4 |
| 4358 | Spectroscopic investigation of the species involved in the rhodium-catalyzed oxidative carbonylation of toluene to toluic acid. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 9903. | 1.3 | 13 |
| 4359 | Tuning the Oxidation Level, the Spin State, and the Degree of Electron Delocalization in Homo- and Heteroleptic Bis(±-diimine)iron Complexes. <i>Journal of the American Chemical Society</i> , 2009, 131, 1208-1221. | 6.6 | 109 |
| 4360 | Theoretical investigation of the molecular and electronic structures and excitation spectra of iron phthalocyanine and its derivatives, FePc and FePcLn (L = Py, CN ^{âˆ’} ; n = 1, 2). <i>Dalton Transactions</i> , 2009, , 5737. | 1.6 | 24 |
| 4361 | Prediction of spin-spin coupling constants in solution based on combined density functional theory/molecular mechanics. <i>Journal of Chemical Physics</i> , 2009, 130, 134508. | 1.2 | 48 |
| 4362 | Assessment of the ϵ -6-31+G** + LANL2DZ ϵ -Mixed Basis Set Coupled with Density Functional Theory Methods and the Effective Core Potential: Prediction of Heats of Formation and Ionization Potentials for First-Row-Transition-Metal Complexes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9843-9851. | 1.1 | 313 |
| 4363 | Antihypertensive Drug Valsartan in Solution and at the AT ₁ Receptor: Conformational Analysis, Dynamic NMR Spectroscopy, <i>in Silico</i> Docking, and Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 726-739. | 2.5 | 39 |
| 4364 | Robust Periodic Hartree-Fock Exchange for Large-Scale Simulations Using Gaussian Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3010-3021. | 2.3 | 254 |
| 4365 | Universal Solvation Model Based on the Generalized Born Approximation with Asymmetric Descreening. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2447-2464. | 2.3 | 120 |
| 4366 | Probing the Electronic and Structural Properties of the Niobium Trimer Cluster and Its Mono- and Dioxides: Nb ₃ O _n ^{âˆ’} and Nb ₃ O _n (n = 0âˆ’2). <i>Journal of Physical Chemistry A</i> , 2009, 113, 3866-3875. | 1.1 | 55 |
| 4367 | Intermolecular Interactions as Actors in Energy-Transfer Processes in Lanthanide Complexes with 2,2âˆ’-Bipyridine. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9265-9277. | 1.2 | 105 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4368 | Unexpected Regioselectivity in the Synthesis of Pyranonaphthoquinone via the Diels-Alder Reaction. <i>Organic Letters</i> , 2009, 11, 4628-4631. | 2.4 | 13 |
| 4369 | Parallel multireference configuration interaction calculations on mini- β -carotenes and β -carotene. <i>Journal of Chemical Physics</i> , 2009, 130, 044708. | 1.2 | 111 |
| 4370 | DFT Calculations on Heterocyclacenes. <i>Organic Letters</i> , 2009, 11, 725-728. | 2.4 | 22 |
| 4371 | Performance of Density Functional Theory for 3d Transition Metal-Containing Complexes: Utilization of the Correlation Consistent Basis Sets. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8607-8614. | 1.1 | 84 |
| 4372 | Calculation of Electronic Circular Dichroism Spectra with Time-Dependent Double-Hybrid Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 767-776. | 1.1 | 133 |
| 4373 | Atomic charge densities generated using an iterative stockholder procedure. <i>Journal of Chemical Physics</i> , 2009, 131, 144101. | 1.2 | 83 |
| 4374 | Parallel Genetic Algorithms for Crystal Structure Prediction: Successes and Failures in Predicting Bicalutamide Polymorphs. <i>Lecture Notes in Computer Science</i> , 2009, , 120-129. | 1.0 | 0 |
| 4375 | NMR tensors in planar hydrocarbons of increasing size. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11404. | 1.3 | 27 |
| 4376 | Validation of the B3LYP/N07D and PBE0/N07D Computational Models for the Calculation of Electronic $\langle i \rangle \langle j \rangle$ -Tensors. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 192-199. | 2.3 | 79 |
| 4377 | Modelling of electron and hole trapping in oxides. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2009, 17, 084004. | 0.8 | 51 |
| 4378 | Computational DFT Study of Ruthenium Tetracarbonyl Polymer. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1084-1090. | 2.3 | 36 |
| 4379 | Orientation of the GM1 ganglioside in Langmuir-Blodgett monolayers: a PM IRRAS and computational study. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 10140. | 1.3 | 24 |
| 4380 | Automatized Parametrization of SCC-DFTB Repulsive Potentials: Application to Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11866-11881. | 1.1 | 69 |
| 4381 | Probing chiral solute-water hydrogen bonding networks by chirality transfer effects: A vibrational circular dichroism study of glycidol in water. <i>Journal of Chemical Physics</i> , 2009, 130, 164506. | 1.2 | 60 |
| 4382 | Gold-Catalyzed [4C+2C] Cycloadditions of Allenedienes, including an Enantioselective Version with New Phosphoramidite-Based Catalysts: Mechanistic Aspects of the Divergence between [4C+3C] and [4C+2C] Pathways. <i>Journal of the American Chemical Society</i> , 2009, 131, 13020-13030. | 6.6 | 258 |
| 4383 | Electronic structure and magnetic properties of a trigonal prismatic Cull ₆ cluster. <i>Dalton Transactions</i> , 2009, , 5924. | 1.6 | 33 |
| 4384 | Enhancing the Photochemical Stability of $\langle i \rangle \langle j \rangle$ -Chelate Boryl Compounds: C-C Bond Formation versus C-C Bond $\langle i \rangle \langle j \rangle$ -Isomerization. <i>Journal of the American Chemical Society</i> , 2009, 131, 14549-14559. | 6.6 | 85 |
| 4385 | A multiresponsive two-arm ferrocene-based chemosensor molecule for selective detection of mercury. <i>Dalton Transactions</i> , 2009, , 2121. | 1.6 | 41 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4386 | H-Bond-Assisted Regioselective (<i>cis</i> -1) Intramolecular Nucleophilic Addition of the Hydroxyl Group to [60]Fullerene. <i>Journal of Organic Chemistry</i> , 2009, 74, 1480-1487. | 1.7 | 37 |
| 4387 | Comparison of Global Reactivity Descriptors Calculated Using Various Density Functionals: A QSAR Perspective. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2744-2753. | 2.3 | 142 |
| 4388 | Charge Transport Parameters and Structural and Electronic Properties of Octathio[8]circulene and Its Plate-like Derivatives. <i>Journal of Physical Chemistry A</i> , 2009, 113, 255-262. | 1.1 | 35 |
| 4389 | Perspective on Diabatic Models of Chemical Reactivity as Illustrated by the Gas-Phase SN2 Reaction of Acetate Ion with 1,2-Dichloroethane. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1-22. | 2.3 | 45 |
| 4390 | Structural Characterization of the (Methanol) ₄ Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10167-10173. | 1.1 | 53 |
| 4391 | Competitive Retro-Cycloaddition Reaction in Fullerene Dimers Connected through Pyrrolidinopyrazolino Rings. <i>Journal of Organic Chemistry</i> , 2009, 74, 8174-8180. | 1.7 | 25 |
| 4392 | Examination of DFT and TDDFT Methods II. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10873-10879. | 1.1 | 19 |
| 4393 | Matching Active Site and Substrate Structures for an RNA Editing Reaction. <i>Journal of the American Chemical Society</i> , 2009, 131, 11882-11891. | 6.6 | 27 |
| 4394 | Deactivation of the Shvo Catalyst by Ammonia: Synthesis, Characterization, and Modeling. <i>Organometallics</i> , 2009, 28, 473-479. | 1.1 | 26 |
| 4395 | A Computational Study of the Mechanism of Addition of Singlet Carbene Analogues to 1,3-Butadiene to Form 1,1-Dimethylmetallacyclopent-3-enes [MMe ₂ C ₄ H ₆ , M = Si, Ge, Sn] and Their Reverse Retro-addition Reactions. <i>Organometallics</i> , 2009, 28, 5612-5622. | 1.1 | 29 |
| 4396 | Competing Mechanistic Channels in the Oxidation of Aldehydes by Ozone. <i>Journal of Organic Chemistry</i> , 2009, 74, 2108-2113. | 1.7 | 36 |
| 4397 | First-principles calculations of defects near a grain boundary in MgO. <i>Physical Review B</i> , 2009, 79, . | 1.1 | 86 |
| 4398 | Metal ion-catalyzed oxidative degradation of Orange II by H ₂ O ₂ . High catalytic activity of simple manganese salts. <i>New Journal of Chemistry</i> , 2009, 33, 34-49. | 1.4 | 115 |
| 4399 | Cooperativity in noncovalent interactions of biologically relevant molecules. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 8440. | 1.3 | 47 |
| 4400 | Pairwise additivity in the nuclear magnetic resonance interactions of atomic xenon. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 2485. | 1.3 | 23 |
| 4401 | ³ J-Selective Cross-Coupling Reactions of Potassium Allyltrifluoroborates with Haloarenes Catalyzed by a Pd(O)/D- <i>t</i> -BPF or Pd(O)/Josiphos ((<i>R,S</i>)-CyPF- <i>t</i> -Bu) Complex: Mechanistic Studies on Transmetalation and Enantioselection. <i>Organometallics</i> , 2009, 28, 152-160. | 1.1 | 79 |
| 4402 | Implementation of a Hybrid DFT Method for Calculating NMR Shieldings Using Slater-Type Orbitals with Spin-Orbital Coupling Included. Applications to ¹⁸⁷ Os, ¹⁹⁵ Pt, and ¹³ C in Heavy-Metal Complexes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11495-11500. | 1.1 | 49 |
| 4403 | Regioselective Intramolecular Nucleophilic Addition of Alcohols to C ₆₀ : One-Step Formation of a <i>cis</i> -1 Bicyclic-Fused Fullerene. <i>Journal of Organic Chemistry</i> , 2009, 74, 6253-6259. | 1.7 | 33 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4404 | Stabilization of gold(I) and gold(III) complexes by pyridil bis{3-hexamethylene-iminylthiosemicarbazone}: spectroscopic, structural and computational study. Dalton Transactions, 2009, , 2731. | 1.6 | 22 |
| 4405 | Can short-range hybrids describe long-range-dependent properties?. Journal of Chemical Physics, 2009, 131, 044108. | 1.2 | 426 |
| 4406 | Carbon-hydrogen vs. carbon-halogen oxidative addition of chlorobenzene by a neutral iridium complex explored by DFT. Dalton Transactions, 2009, , 5933. | 1.6 | 21 |
| 4407 | Screened hybrid density functionals for solid-state chemistry and physics. Physical Chemistry Chemical Physics, 2009, 11, 443-454. | 1.3 | 384 |
| 4408 | Reaction of [60]fullerene with trans-epoxides: a theoretical study. Organic and Biomolecular Chemistry, 2009, 7, 1851. | 1.5 | 5 |
| 4409 | High performance gold nanorods and silver nanocubes in surface-enhanced Raman spectroscopy of pesticides. Physical Chemistry Chemical Physics, 2009, 11, 7491. | 1.3 | 68 |
| 4411 | DFT studies on catalytic properties of isolated and carbon nanotube supported Pd ₉ cluster: adsorption, fragmentation and diffusion of hydrogen. Physical Chemistry Chemical Physics, 2009, 11, 4077. | 1.3 | 34 |
| 4412 | Resonance Raman spectra of β -carotene in solution and in photosystems revisited: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2009, 11, 11471. | 1.3 | 90 |
| 4413 | Assessment of the Accuracy of Theoretical Methods for Calculating ²⁷ Al Nuclear Magnetic Resonance Shielding Tensors of Aquated Aluminum Species. Journal of Physical Chemistry A, 2009, 113, 5138-5143. | 1.1 | 21 |
| 4414 | Optimization and Basis-Set Dependence of a Restricted-Open-Shell Form of B2-PLYP Double-Hybrid Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 9861-9873. | 1.1 | 77 |
| 4415 | Theoretical investigation on the dimerization of the deprotonated aquo ion of Al(H_2O) ₃ in water. Dalton Transactions, 2009, , 521-529. | 1.6 | 19 |
| 4416 | Structure and Properties of Redox Active Self-Assembled Monolayers Formed from Norbornylogous Bridges. Langmuir, 2009, 25, 11090-11096. | 1.6 | 17 |
| 4417 | Adenine and Adenosine Monophosphate (AMP) Gold Binding Interactions Studied by Surface-Enhanced Raman and Infrared Spectroscopies. Journal of Physical Chemistry C, 2009, 113, 14390-14397. | 1.5 | 118 |
| 4418 | Facet-Dependent Electronic Properties of Hexagonal Silicon Nanowires under Progressive Hydroxylation and Surface Reconstruction. Nano Letters, 2009, 9, 1999-2004. | 4.5 | 19 |
| 4419 | Fluorine substituent effects on dihydrogen bonding of transition metal hydrides. Physical Chemistry Chemical Physics, 2009, 11, 7231. | 1.3 | 10 |
| 4420 | The use of nanometer-sized hydrographene species for support material for fuel cell electrode catalysts: a theoretical proposal. Physical Chemistry Chemical Physics, 2009, 11, 8275. | 1.3 | 76 |
| 4421 | Modes of inactivation of trichodiene synthase by a cyclopropane-containing farnesyl diphosphate analog. Organic and Biomolecular Chemistry, 2009, 7, 4101. | 1.5 | 26 |
| 4422 | Benchmark Thermochemistry of the C _{2n} H _{2n+2} Alkane Isomers (n = 2-8) and Performance of DFT and Composite Ab Initio Methods for Dispersion-Driven Isomeric Equilibria. Journal of Physical Chemistry A, 2009, 113, 8434-8447. | 1.1 | 128 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4423 | Photodegradation mechanism of the common non-steroid anti-inflammatory drug diclofenac and its carbazole photoproduct. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4601. | 1.3 | 45 |
| 4424 | Stabilisation of an inorganic digallane by the phosphinobisthiolato P,S,S pincer ligand PPh(2-SC ₆ H ₄) ₂ . <i>New Journal of Chemistry</i> , 2009, 33, 1771. | 1.4 | 17 |
| 4425 | Analytic calculations of nonlinear mixed electric and magnetic frequency-dependent molecular properties using London atomic orbitals: Buckingham birefringence. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 816-825. | 1.3 | 14 |
| 4426 | Experimental and theoretical studies of complexes of [PbmAg] ⁺ (m = 1-4). <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1043. | 1.3 | 7 |
| 4427 | Density Functional Theory in Prediction of Four Stepwise Protonation Constants for Nitrilotripropanoic Acid (NTPA). <i>Journal of Physical Chemistry A</i> , 2009, 113, 3639-3647. | 1.1 | 23 |
| 4428 | Comprehensive Investigation of the Energetics of Pyrimidine Nucleoside Formation in a Model Prebiotic Reaction. <i>Journal of the American Chemical Society</i> , 2009, 131, 16088-16095. | 6.6 | 32 |
| 4429 | Structural Trends Among Nanotubes of Group 13-15 Binary Hydrides. <i>Journal of Physical Chemistry C</i> , 2009, 113, 10065-10069. | 1.5 | 8 |
| 4430 | Methyl Group Dynamics in Polycrystalline and Liquid Ubiquinone Q ₀ Studied by Neutron Scattering. <i>Journal of Physical Chemistry B</i> , 2009, 113, 916-922. | 1.2 | 5 |
| 4431 | Computational Modeling Study on Formation of Acyclic Clavulanate Intermediates in Inhibition of Class A β -Lactamase: Water-Assisted Proton Transfer. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1608-1613. | 1.1 | 2 |
| 4432 | A Comparison of 4 <i>f</i> vs 5 <i>f</i> Metal-Metal Bonds in (CpSiMe ₃) ₃ M ⁺ ECp* (M = Nd, U; E = Al, Ga; Cp* = C ₅ Me ₅): Synthesis, Thermodynamics, Magnetism, and Electronic Structure. <i>Journal of the American Chemical Society</i> , 2009, 131, 13767-13783. | 6.6 | 131 |
| 4433 | Seven-Membered Cyclic Dialkylstannylene and -Plumbylene Compounds Stabilized by Agostic-type B ⁺ H ⁻ •E Interactions [E = Sn, Pb]. <i>Organometallics</i> , 2009, 28, 2211-2217. | 1.1 | 25 |
| 4434 | Multidecker Sandwiches of Silicon-Carbon Clusters. <i>Organometallics</i> , 2009, 28, 4308-4315. | 1.1 | 11 |
| 4435 | Roles of the Ether Oxygen in Hydration of Tetrahydrofuran Studied by IR, NMR, and DFT Calculation Methods. <i>Journal of Physical Chemistry B</i> , 2009, 113, 906-915. | 1.2 | 30 |
| 4436 | Investigation of the Ligand-Field States of the Hexaammine Cobalt(III) Ion with Quantum Chemical Methods. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1061-1067. | 2.3 | 9 |
| 4437 | Synthesis, Characterization, and Physical Properties of Cyclometalated Iridium(III) Complexes with 2-Phenylthiophene or 2-Phenylfuran Ligands. <i>Organometallics</i> , 2009, 28, 6079-6089. | 1.1 | 22 |
| 4438 | Atomization energies of the carbon clusters C _n (n = 2-10) revisited by means of W4 theory as well as density functional, G _n , and CBS methods. <i>Molecular Physics</i> , 2009, 107, 977-990. | 0.8 | 41 |
| 4439 | Structural and electronic properties of gold microclusters: assessment of the localized Hartree-Fock method. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 9160. | 1.3 | 10 |
| 4440 | Polynitrogen/Nanoaluminum Surface Interactions. , 2009, , . | | 0 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4442 | Short cut to 1,2,3-triazole-based p38 MAP kinase inhibitors via [3+2]-cycloaddition chemistry. <i>New Journal of Chemistry</i> , 2009, 33, 1010-1016. | 1.4 | 32 |
| 4443 | Matrix isolation studies and DFT calculations on molecular alkali metal bromates. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 650-654. | 1.3 | 0 |
| 4444 | Divalent carbon atom as the proton acceptor in hydrogen bonding. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5711. | 1.3 | 43 |
| 4445 | Mechanistic behaviour of alkylcobaloximes and imino-oxime complexes related to vitamin B12. <i>Dalton Transactions</i> , 2009, , 2392. | 1.6 | 9 |
| 4446 | Substituent effect on the interaction of aromatic primary amines and diamines with supercritical CO ₂ from infrared spectroscopy and quantum calculations. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5052. | 1.3 | 17 |
| 4447 | Theoretical study of the gas-phase ozonolysis of β -pinene (C ₁₀ H ₁₆). <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5643. | 1.3 | 83 |
| 4448 | Photoinduced linkage isomerism of {RuNO} ₆ complexes with bioligands and related chelators. <i>Dalton Transactions</i> , 2009, , 1034. | 1.6 | 23 |
| 4449 | Synthesis and X-ray characterization of [RhCl(C ₂ H ₄)(P <i>i</i> Pr ₃) ₂]. Multinuclear NMR and DFT investigation of its solid-state and solution reaction with dihydrogen. Ethene and propene hydrogenation by the solid Rh-hydrides. <i>Dalton Transactions</i> , 2009, , 7924. | 1.6 | 9 |
| 4450 | ¹⁹ F spin-spin coupling in peri-difluoronaphthalene. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4136. | 1.3 | 8 |
| 4451 | Theoretical investigation of the gas-phase Mn ⁺ - and Co ⁺ -catalyzed oxidation of benzene by N ₂ O. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4219. | 1.3 | 25 |
| 4452 | Is bis(trifluoromethylsulfonyl)amide an innocent anion? X-Ray structure data and DFT calculations. <i>Dalton Transactions</i> , 2009, , 2795. | 1.6 | 22 |
| 4453 | Monoorganobismuth(III) dihalides containing the new pincer 2,6-{MeN(CH ₂ CH ₂) ₂ NCH ₂ } ₂ C ₆ H ₃ ligand: solution NMR, vibrational and single-crystal X-ray studies. <i>Dalton Transactions</i> , 2009, , 77-84. | 1.6 | 32 |
| 4454 | 1,1- and 1,2-isomers of the diborane(4) compound B ₂ {1,2-(NH) ₂ C ₆ H ₄ } ₂ and a TCNQ Co-crystal of the 1,1-isomer. <i>Dalton Transactions</i> , 2009, , 5348. | 1.6 | 20 |
| 4455 | Unexpected nucleophilic behaviour of free-radicals generated from α -iodoketones. <i>Chemical Communications</i> , 2009, , 2142. | 2.2 | 19 |
| 4456 | Theoretical studies on β -aryl elimination from Rh(I) complexes. <i>Dalton Transactions</i> , 2009, , 5841. | 1.6 | 16 |
| 4457 | Ruthenium based catalysts for olefin hydrosilylation: dichloro(<i>p</i> -cymene)ruthenium and related complexes. <i>Dalton Transactions</i> , 2009, , 5894. | 1.6 | 20 |
| 4458 | Robust normal modes in vibrational circular dichroism spectra. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 6107. | 1.3 | 85 |
| 4459 | Carbon-hydrogen vs. carbon-halogen oxidative addition of chlorobenzene to a cationic iridium(I) system - A density functional theory study. <i>Canadian Journal of Chemistry</i> , 2009, 87, 1460-1469. | 0.6 | 5 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4460 | Finite-temperature effects in enzymatic reactions â€” Insights from QM/MM free-energy simulations. Canadian Journal of Chemistry, 2009, 87, 1322-1337. | 0.6 | 64 |
| 4461 | The Zinc proteome: a tale of stability and functionality. Dalton Transactions, 2009, , 7946. | 1.6 | 71 |
| 4462 | Charge-transport properties of prototype molecular materials for organic electronics based on graphene nanoribbons. Physical Chemistry Chemical Physics, 2009, 11, 2741. | 1.3 | 47 |
| 4463 | The gas-phase ozonolysis of Î²-caryophyllene (C ₁₅ H ₂₄). Part II: A theoretical study. Physical Chemistry Chemical Physics, 2009, 11, 4173. | 1.3 | 66 |
| 4464 | Reactivity of CO ₂ towards Mo[N(R)Ph] ₃ . Dalton Transactions, 2009, , 9266. | 1.6 | 13 |
| 4465 | Density functional theory â€” electron paramagnetic resonance study of gamma-irradiated single crystal of amphi-chloroglyoxime. Radiation Effects and Defects in Solids, 2009, 164, 73-82. | 0.4 | 9 |
| 4466 | The water-benzene interaction: Insight from electronic structure theories. Journal of Chemical Physics, 2009, 130, 154303. | 1.2 | 73 |
| 4467 | A simple nonlocal model for exchange. Journal of Chemical Physics, 2009, 131, 234111. | 1.2 | 20 |
| 4468 | Redox-Switchable Second-Order Nonlinear Optical Responses of Pushâ€”Pull Monotetrathiafulvalene-Metalloporphyrins. Inorganic Chemistry, 2009, 48, 6548-6554. | 1.9 | 103 |
| 4469 | Hydrotrioxides Rather than Cyclic Tetraoxides (Tetraoxolanes) as the Primary Reaction Intermediates in the Low-Temperature Ozonation of Aldehydes. The Case of Benzaldehyde. Journal of Organic Chemistry, 2009, 74, 96-101. | 1.7 | 14 |
| 4470 | Assigning the Stereochemistry of Pairs of Diastereoisomers Using GIAO NMR Shift Calculation. Journal of Organic Chemistry, 2009, 74, 4597-4607. | 1.7 | 224 |
| 4471 | Structure Dependence of Hyperpolarizability in Octopolar Molecules. Journal of Chemical Theory and Computation, 2009, 5, 850-858. | 2.3 | 14 |
| 4472 | On the Stability of Six-Membered-Ring Carbenes and Silylenes. Organometallics, 2009, 28, 5909-5914. | 1.1 | 12 |
| 4473 | Ferrous Iron Reduction of Superoxide, A Proton-Coupled Electron-Transfer Four-Point Test. Journal of Physical Chemistry A, 2009, 113, 1020-1025. | 1.1 | 7 |
| 4474 | A Computational Comparison of Electron Transfer from Reduced Ferredoxin to Flavin Adenine Dinucleotide and a Gold Electrode. Journal of Physical Chemistry B, 2009, 113, 7298-7307. | 1.2 | 2 |
| 4475 | TDDFT diagnostic testing and functional assessment for triazene chromophores. Physical Chemistry Chemical Physics, 2009, 11, 4465. | 1.3 | 145 |
| 4476 | Semiempirical Molecular Dynamics Study of Empty C ₂ (3)-C ₈₂ Fullerene in Neutral and Charged Forms: Geometrical and Spectroscopic Characterization. Journal of Physical Chemistry C, 2009, 113, 19658-19663. | 1.5 | 2 |
| 4477 | Microsolvation of Cysteine: A Density Functional Theory Study. Journal of Physical Chemistry A, 2009, 113, 6172-6181. | 1.1 | 45 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4478 | Steric effects which determine the conformational preferences and stereodynamic processes of aryl fluorenyl ketones. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 1619. | 1.5 | 4 |
| 4479 | Fluoride recognition by a chiral urea receptor linked to a phthalimide chromophore. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 3499. | 1.5 | 37 |
| 4480 | Structures and composition-dependent polarizabilities of open- and closed-shell Ga_n clusters. <i>Physical Review A</i> , 2009, 80, . | 1.0 | 20 |
| 4481 | DFT Study on N ₂ Activation by a Hydride-Bridged Diniobium Complex. N≡N Bond Cleavage Accompanied by H ₂ Evolution. <i>Inorganic Chemistry</i> , 2009, 48, 3875-3881. | 1.9 | 29 |
| 4482 | A density functional study on cationic Au _n Cu _m ⁺ clusters and their monocarbonyls. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 2329. | 1.3 | 33 |
| 4483 | Hydration of Carboxylate Anions: Infrared Spectroscopy of Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2009, 113, 8128-8136. | 1.2 | 39 |
| 4484 | Hybrid density functional theory applied to magnetite: Crystal structure, charge order, and phonons. <i>Physical Review B</i> , 2009, 79, . | 1.1 | 65 |
| 4485 | Reliable Prediction of Charge Transfer Excitations in Molecular Complexes Using Time-Dependent Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2009, 131, 2818-2820. | 6.6 | 729 |
| 4486 | Histidine-Containing Radicals in the Gas Phase. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7347-7366. | 1.2 | 25 |
| 4487 | Crossed-Beam Dynamics, Low-Temperature Kinetics, and Theoretical Studies of the Reaction S(¹ D) + C ₂ H ₄ . <i>Journal of Physical Chemistry A</i> , 2009, 113, 15328-15345. | 1.1 | 38 |
| 4488 | Tuning the Binding Energy of Surfactant to CdSe Nanocrystal: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 3116-3119. | 1.5 | 13 |
| 4489 | Competitive Enantiodifferentiating Anti-Markovnikov Photoaddition of Water and Methanol to 1,1-Diphenylpropene Using A Sensitizing Cyclodextrin Host. <i>Journal of Organic Chemistry</i> , 2009, 74, 6714-6727. | 1.7 | 38 |
| 4490 | Transfer of Noncovalent Chiral Information along an Optically Inactive Helical Peptide Chain: Allosteric Control of Asymmetry of the C-Terminal Site by External Molecule that Binds to the N-Terminal Site. <i>Journal of Organic Chemistry</i> , 2009, 74, 1429-1439. | 1.7 | 61 |
| 4491 | Excited states of Nb ₃ N ₂ and Nb ₃ C ₂ : Density functional theory, CASSCF, and MRCI studies. <i>Journal of Chemical Physics</i> , 2009, 130, 164308. | 1.2 | 5 |
| 4492 | Anions [N(CH ₂) ₃] ⁻ and [ON(CH ₂) ₂] ⁻ are Stable in the Gas Phase, but Can They Be Charge Stripped to Form the Radicals N(CH ₂) ₃ and ON(CH ₂) ₂ ? A Joint Experimental and Theoretical Study. <i>European Journal of Mass Spectrometry</i> , 2009, 15, 91-104. | 0.5 | 1 |
| 4493 | THE INFRARED SPECTRA OF VERY LARGE IRREGULAR POLYCYCLIC AROMATIC HYDROCARBONS (PAHs): OBSERVATIONAL PROBES OF ASTRONOMICAL PAH GEOMETRY, SIZE, AND CHARGE. <i>Astrophysical Journal</i> , 2009, 697, 311-327. | 1.6 | 153 |
| 4495 | Crossed-Beam and Theoretical Studies of the S(¹ D) + C ₂ H ₂ Reaction. <i>Journal of Physical Chemistry A</i> , 2009, 113, 4330-4339. | 1.1 | 28 |
| 4496 | Experimental and Theoretical Evidence for HS ₄ . <i>Journal of Physical Chemistry A</i> , 2009, 113, 14420-14423. | 1.1 | 2 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4497 | Arylation of 3-heterylmethylene-5-arylfuran-2(3H)-thiones. <i>Journal of Chemical Research</i> , 2009, 2009, 68-71. | 0.6 | 4 |
| 4498 | A theoretical study of the dehydration of tertiary butanol in near-critical and supercritical water. <i>Molecular Physics</i> , 2009, 107, 27-35. | 0.8 | 3 |
| 4499 | On Occupied-orbital Dependent Exchange-correlation Functionals: From Local Hybrids to Becke's B05 Model. <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 545-567. | 1.4 | 8 |
| 4500 | Communication: Hilbert-space partitioning of the molecular one-electron density matrix with orthogonal projectors. <i>Journal of Chemical Physics</i> , 2010, 133, 231103. | 1.2 | 9 |
| 4502 | 9-Borafluorenes' NMR spectroscopy and DFT calculations. Molecular structure of 1,2-(2,2-diphenyl)-1,2-diethylidiborane. <i>Collection of Czechoslovak Chemical Communications</i> , 2010, 75, 743-756. | 1.0 | 13 |
| 4503 | Synthesis and Properties of Secondary Thiocarbamoylsilanes. <i>Bulletin of the Chemical Society of Japan</i> , 2010, 83, 52-57. | 2.0 | 8 |
| 4505 | Theoretical Studies on Conformational Features of Poly(lactic acid)Chain Containing a Racemic Unit. <i>Kobunshi Ronbunshu</i> , 2010, 67, 214-223. | 0.2 | 2 |
| 4506 | Organoammonium Salt-Catalyzed Enantioselective Cycloaddition Reactions with $\hat{\pm}$ -(Acyloxy)- or $\hat{\pm}$ -Diacylaminoacroleins. <i>Bulletin of the Chemical Society of Japan</i> , 2010, 83, 313-322. | 2.0 | 18 |
| 4507 | Kinetic Analysis for the Effect of Intramolecular Hydrogen Bonding on Photophysical Properties of <i>i</i> -Hydroxyalkyl-1,8-naphthalimides. <i>Bulletin of the Chemical Society of Japan</i> , 2010, 83, 1067-1073. | 2.0 | 7 |
| 4508 | X-Ray diffraction and vibrational spectroscopic study of 2-chloro-N-{4-[3-(2,5-dimethylphenyl)-3-methylcyclobutyl]-thiazol-2-yl}-acetamide. <i>Crystallography Reports</i> , 2010, 55, 1183-1187. | 0.1 | 2 |
| 4509 | Synthesis, structure, and complexing ability of a novel ligand system, 1-benzyl-2-benzimidazolylhydrazone of pyrrol-2-carbaldehyde. <i>Russian Journal of General Chemistry</i> , 2010, 80, 1689-1696. | 0.3 | 1 |
| 4510 | Physicochemical study of new polydentane ligand systems based on 2,6-diformyl-4-tert-butylphenol. <i>Russian Journal of General Chemistry</i> , 2010, 80, 2329-2336. | 0.3 | 3 |
| 4511 | 2-Acetylbenzimidazole phthalazin-1-ylhydrazone and its complexes with transition metals. <i>Russian Journal of General Chemistry</i> , 2010, 80, 2501-2511. | 0.3 | 9 |
| 4512 | Theoretical studies on the electronic structures and spectra of single silicon-doped SWCNTs. <i>Open Chemistry</i> , 2010, 8, 587-593. | 1.0 | 2 |
| 4513 | Creation of multihole molecular wave packets via strong-field ionization. <i>Physical Review A</i> , 2010, 82, . | 1.0 | 24 |
| 4514 | Third-Generation Hydrogen-Bonding Corrections for Semiempirical QM Methods and Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3808-3816. | 2.3 | 213 |
| 4515 | Basis set effects on the hyperpolarizability of CHCl ₃ : Gaussian-type orbitals, numerical basis sets and real-space grids. <i>Journal of Chemical Physics</i> , 2010, 133, 034111. | 1.2 | 46 |
| 4516 | Performance of Relativistic Effective Core Potentials in DFT Calculations on Actinide Compounds. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1957-1963. | 1.1 | 60 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4517 | DFT Study on the Catalytic Reactivity of a Functional Model Complex for Intradiol-Cleaving Dioxygenases. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5878-5885. | 1.2 | 25 |
| 4518 | Experimental and Computational Study of the Structural and Electronic Properties of $\text{Fe}^{\text{II}}(2,2\text{-bipyridine})(\text{mes})_2$ and $[\text{Fe}^{\text{II}}(2,2\text{-bipyridine})(\text{mes})_2]^{\text{+}}$, a Complex Containing a 2,2-Bipyridyl Radical Anion. <i>Inorganic Chemistry</i> , 2010, 49, 6160-6171. | 1.9 | 57 |
| 4519 | Two-component relativistic density functional theory modeling of the adsorption of element 114(eka-lead) on gold. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4152. | 1.3 | 28 |
| 4520 | Phospha-Macrocyclic Chelates: Electronic Structures and 1,3-Dipolar Cycloadditions. <i>Journal of Organic Chemistry</i> , 2010, 75, 4261-4273. | 1.7 | 41 |
| 4521 | Synthesis, X-ray Structure, Magnetic Resonance, and DFT Analysis of a Soluble Copper(II) Phthalocyanine Lacking C-H Bonds. <i>Inorganic Chemistry</i> , 2010, 49, 8779-8789. | 1.9 | 38 |
| 4522 | On the microwave-assisted synthesis of acylphenothiazine derivatives – Experiment versus theory synergism. <i>Canadian Journal of Chemistry</i> , 2010, 88, 42-49. | 0.6 | 16 |
| 4523 | Design, synthesis, characterisation and chemical reactivity of mixed-ligand platinum(II) oxadiazoline complexes with potential cytotoxic properties. <i>Dalton Transactions</i> , 2010, 39, 7747. | 1.6 | 18 |
| 4524 | Computational Explorations of Mechanisms and Ligand-Directed Selectivities of Copper-Catalyzed Ullmann-Type Reactions. <i>Journal of the American Chemical Society</i> , 2010, 132, 6205-6213. | 6.6 | 324 |
| 4525 | A Transferable H-Bonding Correction for Semiempirical Quantum-Chemical Methods. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 344-352. | 2.3 | 249 |
| 4526 | A consistent and accurate <i>ab initio</i> parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. <i>Journal of Chemical Physics</i> , 2010, 132, 154104. | 1.2 | 35,972 |
| 4527 | Mechanism of electrocatalytic hydrogen production by a di-iron model of iron-iron hydrogenase: A density functional theory study of proton dissociation constants and electrode reduction potentials. <i>Dalton Transactions</i> , 2010, 39, 3093. | 1.6 | 73 |
| 4528 | Comparative Study of Copper- and Silver-Catalyzed Protodecarboxylations of Carboxylic Acids. <i>ChemCatChem</i> , 2010, 2, 430-442. | 1.8 | 139 |
| 4529 | Acceleration of the Rate of the Heck Reaction through UV- and Visible-Light-Induced Palladium(II) Reduction. <i>ChemCatChem</i> , 2010, 2, 1467-1476. | 1.8 | 41 |
| 4530 | Ground and excited electronic states of azobenzene: A quantum Monte Carlo study. <i>Journal of Chemical Physics</i> , 2010, 133, 244301. | 1.2 | 34 |
| 4531 | Enol Tautomers of Watson-Crick Base Pair Models Are Metastable Because of Nuclear Quantum Effects. <i>Journal of the American Chemical Society</i> , 2010, 132, 11510-11515. | 6.6 | 79 |
| 4532 | Optical transitions in semiconducting zigzag carbon nanotubes with small diameters: A first-principles broad-range study. <i>Physical Review B</i> , 2010, 82, . | 1.1 | 14 |
| 4534 | Characterisation of geometric isomers of europium chlorides with 2,2-bipyridine based on X-ray diffraction, luminescence and quantum chemical data. <i>Molecular Physics</i> , 2010, 108, 557-572. | 0.8 | 7 |
| 4535 | Circular Dichroism Tensor of a Triarylmethyl Propeller in Sodium Chlorate Crystals. <i>Journal of the American Chemical Society</i> , 2010, 132, 7454-7465. | 6.6 | 26 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4536 | Effect of Applied Voltage on the Geometrical and Electronic Structures of Dipyrimidinyl-Diphenyl Diblock as a Molecular Diode: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 21728-21735. | 1.5 | 12 |
| 4537 | Structural study of 2-pyridine-derived N(4)-p-tolyl thiosemicarbazone zinc(II) complexes—DFT analysis. <i>Journal of Coordination Chemistry</i> , 2010, 63, 2879-2887. | 0.8 | 2 |
| 4538 | Comparative Theoretical Study on Homopolymerization of α -Olefins by Bis(cyclopentadienyl) Zirconocene and Hafnocene: Elemental Propagation and Termination Reactions between Monomers and Metals. <i>Organometallics</i> , 2010, 29, 1541-1550. | 1.1 | 38 |
| 4539 | Assigning Stereochemistry to Single Diastereoisomers by GIAO NMR Calculation: The DP4 Probability. <i>Journal of the American Chemical Society</i> , 2010, 132, 12946-12959. | 6.6 | 686 |
| 4540 | Nature and Strength of M-S Bonds (M = Au, Ag, and Cu) in Binary Alloy Gold Clusters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9212-9221. | 1.1 | 161 |
| 4541 | Synthesis and Properties of N_7O_7 . <i>Inorganic Chemistry</i> , 2010, 49, 1245-1251. | 1.9 | 15 |
| 4542 | ^{13}C Chemical Shift Tensors in Hypoxanthine and 6-Mercaptopurine: Effects of Substitution, Tautomerism, and Intermolecular Interactions. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1985-1995. | 1.1 | 33 |
| 4543 | Patterns of π -electron delocalization in aromatic and antiaromatic organic compounds in the light of Hückel's $4n + 2$ rule. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7126. | 1.3 | 38 |
| 4544 | Singlet and triplet potential surfaces for the $O_2 + C_2H_4$ reaction. <i>Journal of Chemical Physics</i> , 2010, 133, 184306. | 1.2 | 17 |
| 4545 | Role of quantum chemical calculations in molecular biophysics with a historical perspective. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 121-144. | 0.5 | 6 |
| 4546 | A DFT study of uracil and 5-bromouracil in nanodroplets. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 233-244. | 0.5 | 31 |
| 4547 | Adenine versus guanine quartets in aqueous solution: dispersion-corrected DFT study on the differences in π -stacking and hydrogen-bonding behavior. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 245-252. | 0.5 | 123 |
| 4548 | Computational methods for analysis of an unsaturated carbocycle: heptafulvene. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 55-73. | 0.5 | 8 |
| 4549 | The optimum contraction of basis sets for calculating spin-spin coupling constants. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 371-382. | 0.5 | 125 |
| 4550 | Fluorene-based oligomers as red light-emitting materials: a density functional theory study. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 305-314. | 0.5 | 3 |
| 4551 | Theoretical investigations of the charge transfer properties of anthracene derivatives. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 587-594. | 0.5 | 28 |
| 4552 | The physical chemistry of $[M(H_2O)_4(NO_3)_2]$ ($M = Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}$) complexes: computational studies of their structure, energetics and the topological properties of the electron density. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 711-725. | 0.5 | 33 |
| 4553 | Overcoming systematic DFT errors for hydrocarbon reaction energies. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 429-442. | 0.5 | 51 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 4554 | Derivation of the supermolecular interaction energy from the monomer densities in the density functional theory. <i>Chemical Physics Letters</i> , 2010, 486, 160-165. | 1.2 | 20 |
| 4555 | Optimal control design of laser pulses for mode specific vibrational excitation in an enzyme-substrate complex. <i>Chemical Physics Letters</i> , 2010, 491, 230-236. | 1.2 | 3 |
| 4556 | Structural reciprocity effect in binary silicon-bismuth clusters. <i>Chemical Physics Letters</i> , 2010, 493, 45-48. | 1.2 | 7 |
| 4557 | The K-band $\hat{\lambda}$ max values of the ultraviolet-visible spectra of some hydrazones in ethanol by a TD-DFT/PCM approach. <i>Chemical Physics Letters</i> , 2010, 494, 198-201. | 1.2 | 4 |
| 4558 | Anchoring Pd nanoclusters onto pristine and functionalized single-wall carbon nanotubes: A combined DFT and experimental study. <i>Chemical Physics Letters</i> , 2010, 497, 103-107. | 1.2 | 34 |
| 4559 | Microsolvation of uracil anion radical in aqueous solution: a QM/MM study. <i>Chemical Physics Letters</i> , 2010, 500, 104-110. | 1.2 | 7 |
| 4560 | Unprecedented triphosphinine iron interactions: Intramolecular electron transfer, reactivity round a corner, and a low-activated ring element exchange reaction. <i>Comptes Rendus Chimie</i> , 2010, 13, 1203-1212. | 0.2 | 14 |
| 4561 | Revisiting the electrochemical formation, stability and structure of radical and biradical anionic structures in dinitrobenzenes. <i>Electrochimica Acta</i> , 2010, 55, 8325-8335. | 2.6 | 12 |
| 4562 | Unexpected reactivity resulting from modifications of the ligand periphery: Synthesis, structure, and spectroscopic properties of iron complexes of new tripodal N-heterocyclic carbene (NHC) ligands. <i>Inorganica Chimica Acta</i> , 2010, 364, 226-237. | 1.2 | 24 |
| 4563 | Theoretical studies on structures and electronic spectra of linear $HC_{2n+1}H^+$ ($n=2-7$). <i>International Journal of Mass Spectrometry</i> , 2010, 290, 113-119. | 0.7 | 8 |
| 4564 | A DFT study of electronic structures of thiophene-based organosilicon compounds. <i>Chemical Physics</i> , 2010, 367, 167-174. | 0.9 | 9 |
| 4565 | The conductance and stability of fused dithia-heterocyclic compounds contacted with gold and platinum electrodes. <i>Chemical Physics</i> , 2010, 375, 67-72. | 0.9 | 7 |
| 4566 | Molecular first order hyperpolarizability and vibrational spectral investigation of Warfarin sodium. <i>Chemical Physics</i> , 2010, 378, 88-102. | 0.9 | 11 |
| 4567 | Chromophore-specific theoretical spectroscopy: From subsystem density functional theory to mode-specific vibrational spectroscopy. <i>Physics Reports</i> , 2010, 489, 1-87. | 10.3 | 118 |
| 4568 | Control of degradation of polypropylene during its radical functionalisation with furan and thiophene derivatives. <i>Polymer Degradation and Stability</i> , 2010, 95, 298-305. | 2.7 | 31 |
| 4569 | Ab initio HF and DFT simulations, FT-IR and FT-Raman vibrational analysis of $\hat{\lambda}$ -chlorotoluene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 77, 150-159. | 2.0 | 48 |
| 4570 | Experimental (FT-IR and FT-RS) and theoretical (DFT) studies of molecular structure and internal modes of $[Mn(NH_3)_6](NO_3)_2$. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 77, 402-410. | 2.0 | 16 |
| 4571 | DFT approach to reaction mechanisms through molecular complexes. The case of an organo-catalysed nucleosidation reaction. <i>Computational and Theoretical Chemistry</i> , 2010, 944, 43-52. | 1.5 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4572 | On the nature of halogen bond – The Kohn–Sham molecular orbital approach. <i>Computational and Theoretical Chemistry</i> , 2010, 945, 89-92. | 1.5 | 122 |
| 4573 | Theoretical study of weak CC double bond coordination in a gold (I) catalyst precursor. <i>Computational and Theoretical Chemistry</i> , 2010, 957, 21-25. | 1.5 | 33 |
| 4574 | A computational study of axial vs. equatorial preferences of phenyl-substituted phosphorinane oxides. <i>Computational and Theoretical Chemistry</i> , 2010, 958, 133-136. | 1.5 | 3 |
| 4575 | FT-IR, FT-Raman spectra, density functional computations of the vibrational spectra and molecular geometry of 2-hydroxyquinoxaline. <i>Journal of Molecular Structure</i> , 2010, 963, 194-201. | 1.8 | 11 |
| 4576 | Synthesis, spectroscopic, molecular and computational structure characterizations of (E)-2-ethoxy-6-[(phenylimino)methyl]phenol. <i>Journal of Molecular Structure</i> , 2010, 963, 211-218. | 1.8 | 41 |
| 4577 | Molecular structure and vibrational spectrum of [Mg((CH ₃) ₂ SO) ₆](ClO ₄) ₂ studied by infrared and Raman spectroscopies and DFT computations. <i>Journal of Molecular Structure</i> , 2010, 970, 139-146. | 1.8 | 22 |
| 4578 | Polyamines. IV. Spectroscopic properties of N,N-bis-(1,8-naphthalenedicarboximidopropyl)-N-propylamine and supramolecular interactions in its crystals. <i>Journal of Molecular Structure</i> , 2010, 979, 165-171. | 1.8 | 1 |
| 4579 | Synthesis, spectroscopic characterization and X-ray structures of five-coordinate diorganotin(IV) complexes containing 5-hydroxypyrazoline derivatives as ligands. <i>Journal of Molecular Structure</i> , 2010, 981, 46-53. | 1.8 | 6 |
| 4580 | Spectroscopic and theoretical studies of some 2-ethylsulfinyl-(4- ² -substituted)-phenylthioacetates. <i>Journal of Molecular Structure</i> , 2010, 981, 93-102. | 1.8 | 3 |
| 4581 | Spectroscopic, molecular structure characterizations and quantum chemical computational studies of (E)-5-(diethylamino)-2-[(2-fluorophenylimino)methyl]phenol. <i>Journal of Molecular Structure</i> , 2010, 984, 214-220. | 1.8 | 23 |
| 4582 | Structure of 6-hydroxy-1-methylquinolinium chloride hydrate studied by X-ray, DFT calculations, FTIR and NMR spectroscopies. <i>Journal of Molecular Structure</i> , 2010, 984, 359-370. | 1.8 | 7 |
| 4583 | A combined computational and experimental investigation of the [2Fe–2S] cluster in biotin synthase. <i>Journal of Biological Inorganic Chemistry</i> , 2010, 15, 203-212. | 1.1 | 10 |
| 4584 | Efficient multi-scale computation of products of orbitals in electronic structure calculations. <i>Computing and Visualization in Science</i> , 2010, 13, 397-408. | 1.2 | 3 |
| 4585 | Phosphane-stabilized gold clusters: investigation of the stability of [Au ₁₃ (PMe ₂ Ph) ₁₀ Cl ₂] ³⁺ . <i>Journal of Molecular Modeling</i> , 2010, 16, 505-512. | 0.8 | 6 |
| 4586 | A B3LYP and MP2 theoretical investigation into host-guest interaction between calix[4]arene and Li ⁺ or Na ⁺ . <i>Journal of Molecular Modeling</i> , 2010, 16, 589-598. | 0.8 | 11 |
| 4587 | Quantum chemical investigation of intramolecular thione-thiol tautomerism of 1,2,4-triazole-3-thione and its disubstituted derivatives. <i>Journal of Molecular Modeling</i> , 2010, 16, 841-855. | 0.8 | 22 |
| 4588 | Theoretical insights into the trends in molecular properties of HCY, HSiY and HGeY molecules where Y = N, P, As. <i>Journal of Molecular Modeling</i> , 2010, 16, 1075-1084. | 0.8 | 3 |
| 4589 | Theoretical investigation of the ring opening process of verdoheme to biliverdin in the presence of dioxygen. <i>Journal of Molecular Modeling</i> , 2010, 16, 1401-1413. | 0.8 | 8 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4590 | Density-functional calculations for large systems: Can GGA functionals Be competitive with hybrid functionals?. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2010, 2, 163-168. | 2.2 | 10 |
| 4591 | Theoretical studies of vibrationally resolved absorption and emission spectra: From a single chromophore to multichromophoric oligomers/aggregates. <i>Science China Chemistry</i> , 2010, 53, 297-309. | 4.2 | 18 |
| 4592 | A first-principles investigation into the hydrogen bond interaction in \hat{I}^2 -HMX. <i>Science China: Physics, Mechanics and Astronomy</i> , 2010, 53, 1080-1085. | 2.0 | 6 |
| 4593 | Theoretical studies on electronic spectroscopy and dynamics with the real-time time-dependent density functional theory. <i>Frontiers of Chemistry in China: Selected Publications From Chinese Universities</i> , 2010, 5, 11-28. | 0.4 | 10 |
| 4594 | Determining symmetry changes during a chemical reaction: the case of diazene isomerization. <i>Journal of Mathematical Chemistry</i> , 2010, 47, 1274-1286. | 0.7 | 18 |
| 4595 | An AB Initio Study of the Electronic and Geometric Structure of BIS-of Dipivaloylmethane With Manganese, IRON, and Cobalt. <i>Journal of Structural Chemistry</i> , 2010, 51, 622-634. | 0.3 | 4 |
| 4596 | Polarizable Continuum Studies on Methyl and Ethyl Substituted 2,4-Pentanedione. <i>Journal of Solution Chemistry</i> , 2010, 39, 559-565. | 0.6 | 0 |
| 4597 | Selected applications of perturbed angular correlation of \hat{I}^3 -rays (PAC) spectroscopy in biochemistry. <i>Hyperfine Interactions</i> , 2010, 197, 255-267. | 0.2 | 7 |
| 4598 | Modeling the structure and vibrational spectra for oxouranium dichloride monomer and dimer. <i>Journal of Applied Spectroscopy</i> , 2010, 77, 626-630. | 0.3 | 0 |
| 4599 | How the energy evaluation method used in the geometry optimization step affect the quality of the subsequent QSAR/QSPR models. <i>Journal of Computer-Aided Molecular Design</i> , 2010, 24, 17-22. | 1.3 | 9 |
| 4600 | The tunability of the electronic structures for poly(carbosilylsilanes): a theoretical study. <i>Structural Chemistry</i> , 2010, 21, 583-592. | 1.0 | 2 |
| 4601 | Study of cis \leftrightarrow trans isomerization mechanism of 3,3 \hat{I}^2 -azobenzene disulphonate in the lowest singlet and triplet electronic states by density functional theory. <i>Structural Chemistry</i> , 2010, 21, 817-825. | 1.0 | 1 |
| 4602 | Synthesis, spectroscopic characterization, crystal structures, and theoretical studies of (E)-2-(2,4-dimethoxybenzylidene)thiosemicarbazone and (E)-2-(2,5-dimethoxybenzylidene)thiosemicarbazone. <i>Structural Chemistry</i> , 2010, 21, 995-1003. | 1.0 | 14 |
| 4603 | Theoretical study on a new kind of thienyl-functionalized polysilane. <i>Structural Chemistry</i> , 2010, 21, 1263-1271. | 1.0 | 8 |
| 4604 | 7-Ethyl-2,3,5,6,8-pentahydroxy-1,4-naphthoquinone (echinochrome A): a DFT study of the antioxidant mechanism 2.* The structure of monosodium salts of echinochrome A and their reactions with the hydroperoxyl radical. <i>Russian Chemical Bulletin</i> , 2010, 59, 43-54. | 0.4 | 2 |
| 4605 | 7-Ethyl-2,3,5,6,8-pentahydroxy-1,4-naphthoquinone (echinochrome A): a DFT study of the antioxidant mechanism. <i>Russian Chemical Bulletin</i> , 2010, 59, 2185-2202. | 0.4 | 2 |
| 4606 | A new chromium (III) complex containing N-(2-pyridylmethyl)-2-pyrazinecarboxamide, (NPyPzCa): Synthesis, molecular and crystal structure and theoretical electron density analysis. <i>Solid State Sciences</i> , 2010, 12, 1960-1965. | 1.5 | 3 |
| 4607 | Kinetics and mechanism of inhibition of serine esterases by fluorinated aminophosphonates. <i>Chemico-Biological Interactions</i> , 2010, 187, 177-184. | 1.7 | 26 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4608 | Influence of Al ₂ O ₃ on the performance of CeO ₂ used as catalyst in the direct carboxylation of methanol to dimethylcarbonate and the elucidation of the reaction mechanism. Journal of Catalysis, 2010, 269, 44-52. | 3.1 | 113 |
| 4609 | Evaluation of a Combined Quantum Chemical Method Used in Calculating O-H Bond Dissociation Enthalpy. Chinese Journal of Chemistry, 2001, 19, 657-661. | 2.6 | 24 |
| 4610 | Theoretical study on the antioxidant activity of curcumin. Chinese Journal of Chemistry, 2004, 22, 827-830. | 2.6 | 23 |
| 4611 | Synthesis and <i>in vitro</i> Anticancer Activity of Octahedral Platinum(IV) Complexes with Cyclohexyl-Functionalized Ethylenediamine-Diacetate-Type Ligands. ChemMedChem, 2010, 5, 881-889. | 1.6 | 48 |
| 4612 | The Role of Fluorine Substitution in Biphenyl Methylene Imidazole-Type CYP17 Inhibitors for the Treatment of Prostate Carcinoma. ChemMedChem, 2010, 5, 899-910. | 1.6 | 35 |
| 4613 | Two-, One-, and Zero-Dimensional Elemental Nanostructures Based on Ge ₉ -Clusters. ChemPhysChem, 2010, 11, 1944-1950. | 1.0 | 29 |
| 4614 | The X1s Method for Accurate Bond Dissociation Energies. ChemPhysChem, 2010, 11, 2561-2567. | 1.0 | 24 |
| 4615 | Tunable Electronic Properties of a Proton-Responsive N, N-Dimethylaminoazobenzene Fullerene (C ₆₀) Dyad. ChemPhysChem, 2010, 11, 3645-3655. | 1.0 | 11 |
| 4616 | Experimental and Theoretical Conformational Analysis of 5-Benzylimidazolidinone Derivatives as a Playground™ for Studying Dispersion Interactions and a Windshield Wiper™ Effect in Organocatalysis. Helvetica Chimica Acta, 2010, 93, 1-16. | 1.0 | 59 |
| 4617 | Excess electron is trapped in a large single molecular cage C ₆₀ F ₆₀ . Journal of Computational Chemistry, 2010, 31, 195-203. | 1.5 | 49 |
| 4618 | <i>Ab initio</i> periodic study of the conformational behavior of glycine helical homopeptides. Journal of Computational Chemistry, 2010, 31, 1777-1784. | 1.5 | 11 |
| 4619 | Modeling environmental effects on charge density distributions in polar organometallics: Validation of embedded cluster models for the methyl lithium crystal. Journal of Computational Chemistry, 2010, 31, 2568-2576. | 1.5 | 12 |
| 4620 | Accurate prediction of enthalpies of formation for a large set of organic compounds. Journal of Computational Chemistry, 2010, 31, 2585-2592. | 1.5 | 2 |
| 4621 | Water Dissociation and Dioxygen Binding in Phenylalanine Hydroxylase. European Journal of Inorganic Chemistry, 2010, 2010, 351-356. | 1.0 | 5 |
| 4622 | A Selective Chromogenic and Fluorescent Molecular Probe for Yb ^{III} -Based on a Bichromophoric Azadiene. European Journal of Inorganic Chemistry, 2010, 2010, 697-703. | 1.0 | 11 |
| 4623 | Redox Processes Involved in the Synthesis and Reactivity of Oxazolinylthiophenolato Complexes of Iron(II)/(III). European Journal of Inorganic Chemistry, 2010, 2010, 2476-2487. | 1.0 | 5 |
| 4624 | Trapped in a Complex: the 1,2,4,5-tetrakis(tetramethylguanidino)benzene Radical Cation (ttmgb ⁺) with a Bisallylic Structure. European Journal of Inorganic Chemistry, 2010, 2010, 3102-3108. | 1.0 | 38 |
| 4625 | Mesomerization of <i>S</i> ₄ -Symmetric Tetrahedral Chelate Complex [In ₄ (L ³) ₄]: First-Time Monitored by Temperature-Dependent ¹ H NMR Spectroscopy. European Journal of Inorganic Chemistry, 2010, 2010, 2903-2906. | 1.0 | 32 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 4626 | Mono- and Dinuclear Ni ^{II} and Co ^{II} Complexes that Feature Chelating Guanidine Ligands: Structural Characteristics and Molecular Magnetism. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 4770-4782. | 1.0 | 36 |
| 4627 | Epoxidation of Alkenes with H ₂ O ₂ Catalyzed by Ditungstenium-Containing 19 ^{Tungstodiarsenate(III)} : Experimental and Theoretical Studies. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 5312-5317. | 1.0 | 42 |
| 4628 | Kinetic Studies on the Reactions of Different Bifunctional Platinum(II) Complexes with Selected Nucleophiles. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 5439-5445. | 1.0 | 35 |
| 4629 | Density Functional Theory Studies of [Fe(O)2L] ₂ ⁺ : What is the Role of the Spectator Ligand L with Different Coordination Numbers?. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 5113-5123. | 1.0 | 4 |
| 4630 | Recent Advances in Stereodynamics and Conformational Analysis by Dynamic NMR and Theoretical Calculations. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 2035-2056. | 1.2 | 108 |
| 4631 | Experimental and Theoretical Studies of a One-Flask Synthesis of 3H-1-Benzazepines from 2-Haloanilines and α,β -Unsaturated Ketones. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 2363-2371. | 1.2 | 6 |
| 4632 | Theoretical Study on Hetero-Diels-Alder Reaction of Butadiene with Benzaldehyde Catalyzed by Chiral In ^{III} Complexes. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 3867-3875. | 1.2 | 6 |
| 4633 | Rearrangements of N-Heterocyclic Carbenes of Pyrazole to 4-Aminoquinolines and Benzoquinolines. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 4296-4305. | 1.2 | 31 |
| 4634 | Theoretical Investigations towards the Staudinger Reaction Catalyzed by N-Heterocyclic Carbene: Mechanism and Stereoselectivity. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 6249-6255. | 1.2 | 23 |
| 4635 | Silicon Atom Substitution Enhances Interchain Packing in a Thiophene-Based Polymer System. <i>Advanced Materials</i> , 2010, 22, 371-375. | 11.1 | 352 |
| 4636 | Enantioselective Copper-Catalysed Allylic Alkylation of Cinnamyl Chlorides by Grignard Reagents using Chiral Phosphine-Phosphite Ligands. <i>Advanced Synthesis and Catalysis</i> , 2010, 352, 2023-2031. | 2.1 | 50 |
| 4637 | Molecular dynamics simulation of desulfurization by ionic liquids. <i>AIChE Journal</i> , 2010, 56, 2983-2996. | 1.8 | 47 |
| 4639 | Determination of the absolute configurations of synthetic daunorubicin analogues using vibrational circular dichroism spectroscopy and density functional theory. <i>Chirality</i> , 2010, 22, 734-743. | 1.3 | 13 |
| 4640 | Solvent-Dependent Dihydrogen/Dihydride Stability for [Mo(CO)(Cp*)H ₂ (PMe ₃) ₂] ⁺ [BF ₄] ⁻ Determined by Multiple Solvent-Anion-Cation Non-Covalent Interactions. <i>Chemistry - A European Journal</i> , 2010, 16, 189-201. | 1.7 | 31 |
| 4641 | Sandwich Compounds of Transition Metals with Cyclopolyenes and Isolobal Boron Analogues. <i>Chemistry - A European Journal</i> , 2010, 16, 2272-2281. | 1.7 | 15 |
| 4642 | Ligand-Exchange Processes on Solvated Zinc Cations: Water Exchange on [Zn(H ₂ O) ₄ (L)] ²⁺ (L = Heterocyclic Ligand). <i>Chemistry - A European Journal</i> , 2010, 16, 7300-7308. | 1.7 | 12 |
| 4643 | Two-Photon Absorption Circular Dichroism: A New Twist in Nonlinear Spectroscopy. <i>Chemistry - A European Journal</i> , 2010, 16, 3504-3509. | 1.7 | 69 |
| 4644 | Determination of the Absolute Configuration of Pentacoordinate Chiral Phosphorus Compounds in Solution by Using Vibrational Circular Dichroism Spectroscopy and Density Functional Theory. <i>Chemistry - A European Journal</i> , 2010, 16, 2518-2527. | 1.7 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4645 | A Computational Study of the Olefin Epoxidation Mechanism Catalyzed by Cyclopentadienyloxidomolybdenum(VI) Complexes. <i>Chemistry - A European Journal</i> , 2010, 16, 2147-2158. | 1.7 | 84 |
| 4646 | Spin Coupling in Roussin's Red and Black Salts. <i>Chemistry - A European Journal</i> , 2010, 16, 10397-10408. | 1.7 | 32 |
| 4647 | Scission of Carbon Monoxide Using TaR ₃ , R=(N <i>t</i> Bu)Ph or OSi(<i>t</i> Bu) ₃ : A DFT Investigation. <i>Chemistry - A European Journal</i> , 2010, 16, 8117-8132. | 1.7 | 7 |
| 4648 | Tuning the Magnetic Moment of [Ru ₂ (DPHF) ₃ (O ₂ CMe)L] ⁺ Complexes (DPHF= <i>N</i> , <i>N</i> â€²â€²Diphenylformamidinate): A Theoretical Explanation of the Axial Ligand Influence. <i>Chemistry - A European Journal</i> , 2010, 16, 6203-6211. | 1.7 | 25 |
| 4649 | Asymmetric Hydrogenation with Highly Active IndolPhosâ€“Rh Catalysts: Kinetics and Reaction Mechanism. <i>Chemistry - A European Journal</i> , 2010, 16, 6509-6517. | 1.7 | 36 |
| 4650 | Metalâ€“Arene Interactions in Dialkylbiarylphosphane Complexes of Copper, Silver, and Gold. <i>Chemistry - A European Journal</i> , 2010, 16, 5324-5332. | 1.7 | 142 |
| 4651 | Comparison of Thiopheneâ€“Pyrrole Oligomers with Oligothiophenes: A Joint Experimental and Theoretical Investigation of Their Structural and Spectroscopic Properties. <i>Chemistry - A European Journal</i> , 2010, 16, 6866-6876. | 1.7 | 27 |
| 4652 | Spectroscopic Implications of the Electron Donorâ€“Acceptor Effect in the Photoactive Yellow Protein Chromophore. <i>Chemistry - A European Journal</i> , 2010, 16, 11977-11984. | 1.7 | 20 |
| 4653 | Density Functional Calculations of ⁵⁵ Mn, ¹⁴ N and ¹³ C Electron Paramagnetic Resonance Parameters Support an Energetically Feasible Model System for the S ₂ State of the Oxygenâ€“Evolving Complex of Photosystem II. <i>Chemistry - A European Journal</i> , 2010, 16, 10424-10438. | 1.7 | 73 |
| 4654 | On the Mechanism of Rutheniumâ€“Catalyzed Formation of Hydrogen from Alcohols: A DFT Study. <i>Chemistry - A European Journal</i> , 2010, 16, 13487-13499. | 1.7 | 33 |
| 4655 | Competitive and Selective Csp ³ â€“Br versus Csp ² â€“Br Bond Activation in Palladiumâ€“Catalysed Suzuki Crossâ€“Coupling: An Experimental and Theoretical Study of the Role of Phosphine Ligands. <i>Chemistry - A European Journal</i> , 2010, 16, 13390-13397. | 1.7 | 65 |
| 4656 | DFT Investigation of the Palladiumâ€“Catalyzed Eneâ€“Yne Coupling. <i>Chemistry - A European Journal</i> , 2010, 16, 9494-9501. | 1.7 | 15 |
| 4657 | Sulfur Ylide Promoted Synthesis of Nâ€“Protected Aziridines: A Combined Experimental and Computational Approach. <i>Chemistry - A European Journal</i> , 2010, 16, 11744-11752. | 1.7 | 23 |
| 4658 | Characterization, Synthesis and Selfâ€“Aggregation of (âˆ)â€“Alternarolactam: A New Fungal Cytotoxin with Cyclopentenone and Isoquinolinone Scaffolds. <i>Chemistry - A European Journal</i> , 2010, 16, 14479-14485. | 1.7 | 30 |
| 4662 | The Syntheses and Structure of the Vanadium(IV) and Vanadium(V) Binary Azides V(N ₃) ₄ , [V(N ₃) ₃] ₆ ^{2âˆ} , and [V(N ₃) ₃] ₆ ^{âˆ} . <i>Angewandte Chemie - International Edition</i> , 2010, 49, 8008-8012. | 7.2 | 34 |
| 4663 | Tuning the <i>cis</i> / <i>trans</i> Conformer Ratio of Xaaâ€“Pro Amide Bonds by Intramolecular Hydrogen Bonds: The Effect on PPII Helix Stability. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 6324-6327. | 7.2 | 98 |
| 4664 | Monomeric Organoantimony(III) and Organobismuth(III) Compounds Stabilized by an NCN Chelating Ligand: Syntheses and Structures. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 5468-5471. | 7.2 | 152 |
| 4665 | Synthesis, characterization and biological studies of alkenylâ€“substituted titanocene(IV) carboxylate complexes. <i>Applied Organometallic Chemistry</i> , 2010, 24, 656-662. | 1.7 | 19 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4666 | Conformations and properties of the L-tryptophyl-containing peptides in solution, depending on the pH—Theoretical study vs. experiments. <i>Biopolymers</i> , 2010, 93, 727-734. | 1.2 | 32 |
| 4667 | Degradation of poly(ethylene glycol) by electrolysis during the Cu electroplating: A combined experimental and density functional theory study. <i>Journal of Applied Polymer Science</i> , 2010, 117, 2083-2089. | 1.3 | 23 |
| 4668 | Spectroscopic investigations and computational study of 2-acetyl(4-bromophenyl)carbamoyl-4-chlorophenyl acetate. <i>Journal of Raman Spectroscopy</i> , 2010, 41, 707-716. | 1.2 | 36 |
| 4669 | Detailed analysis of the charge transfer complex N,N-dimethylaniline-SO ₂ by Raman spectroscopy and density functional theory calculations. <i>Journal of Raman Spectroscopy</i> , 2010, 41, 771-775. | 1.2 | 20 |
| 4670 | Molecular structure, vibrational spectroscopic studies and NBO analysis of the 3,5-dichlorophenylboronic acid molecule by the density functional method. <i>Journal of Raman Spectroscopy</i> , 2010, 41, 1379-1387. | 1.2 | 28 |
| 4671 | A study of the cesium cation bonding to carboxylate anions by the kinetic method and quantum chemical calculations. <i>Journal of Mass Spectrometry</i> , 2010, 45, 520-527. | 0.7 | 12 |
| 4672 | Electron predators are hydrogen atom traps. Effects of aryl groups on N-C ₁ bond dissociations of peptide radicals. <i>Journal of Mass Spectrometry</i> , 2010, 45, 1280-1290. | 0.7 | 12 |
| 4673 | Systematic MALDI-TOF CID Investigation on Different Substituted mPEG 2000. <i>Macromolecular Chemistry and Physics</i> , 2010, 211, 677-684. | 1.1 | 23 |
| 4674 | Organoboron Polymers for Photovoltaic Bulk Heterojunctions. <i>Macromolecular Rapid Communications</i> , 2010, 31, 1281-1286. | 2.0 | 58 |
| 4675 | EPR study of gamma-irradiated single crystal 4-phenylsemicarbazide. <i>Radiation Physics and Chemistry</i> , 2010, 79, 863-869. | 1.4 | 20 |
| 4676 | Ab initio Hartree-Fock and density functional theory study on characterization of 3-(5-methylthiazol-2-ylidiazonyl)-2-phenyl-1H-indole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 75, 1362-1369. | 2.0 | 52 |
| 4677 | Approximate solution of the mode-mode coupling integral: Application to cytosine and its deuterated derivative. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 77, 446-456. | 2.0 | 10 |
| 4678 | FTIR and FT Raman, molecular geometry, vibrational assignments, ab initio and density functional theory calculations for 1,5-methylnaphthalene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 77, 1099-1107. | 2.0 | 34 |
| 4679 | Amino acid influence on copper binding to peptides: Cysteine versus arginine. <i>Journal of the American Society for Mass Spectrometry</i> , 2010, 21, 522-533. | 1.2 | 43 |
| 4680 | Backbone and side-chain specific dissociations of z ions from non-tryptic peptides. <i>Journal of the American Society for Mass Spectrometry</i> , 2010, 21, 1279-1295. | 1.2 | 47 |
| 4681 | Surface behavior of a model surfactant: A theoretical simulation study. <i>Journal of Colloid and Interface Science</i> , 2010, 348, 159-166. | 5.0 | 17 |
| 4682 | Experimental and computational study of the energetics of 5- and 6-aminoindazole. <i>Journal of Chemical Thermodynamics</i> , 2010, 42, 1240-1247. | 1.0 | 6 |
| 4683 | Diorganotin(IV) N-acetyl-L-cysteinate complexes: Synthesis, solid state, solution phase, DFT and biological investigations. <i>Journal of Inorganic Biochemistry</i> , 2010, 104, 750-758. | 1.5 | 20 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4684 | Common basis for the mechanism of metallo and non-metallo KDO8P synthases. <i>Journal of Inorganic Biochemistry</i> , 2010, 104, 1267-1275. | 1.5 | 5 |
| 4685 | Computational study of the properties and metathesis activity of Mo methylidene species in HZSM-5 zeolite. <i>Journal of Molecular Catalysis A</i> , 2010, 316, 106-111. | 4.8 | 22 |
| 4686 | Nanocrystalline ZSM-5: A catalyst with high activity and selectivity for epoxide rearrangement reactions. <i>Journal of Molecular Catalysis A</i> , 2010, 318, 68-74. | 4.8 | 27 |
| 4687 | Polyamines. III. Spectroscopic properties of N,N-bis-(phthalimidopropyl)-N-octylamine and supramolecular interactions in its crystals. <i>Journal of Molecular Structure</i> , 2010, 967, 34-41. | 1.8 | 4 |
| 4688 | Theoretical and experimental study on the reactions between 3,5-di-O-p-toluoyl-d-2-deoxyribose chloride and alcohols. <i>Journal of Molecular Structure</i> , 2010, 977, 1-5. | 1.8 | 2 |
| 4689 | Structure of 3-aminopyridine betaine hydrochloride studied by X-ray diffraction, DFT calculations, FTIR and NMR spectroscopy. <i>Journal of Molecular Structure</i> , 2010, 979, 12-21. | 1.8 | 8 |
| 4690 | Conformational preferences for some 2-substituted N-methoxy-N-methylacetamides through spectroscopic and theoretical studies. <i>Journal of Molecular Structure</i> , 2010, 977, 106-116. | 1.8 | 2 |
| 4691 | The roles of ligands proton affinity, π -back donation and metal fragment hardness on the Au-N bond in N-donor heterocycles gold(III) complexes. <i>Polyhedron</i> , 2010, 29, 767-772. | 1.0 | 8 |
| 4692 | Synthesis of neutral gold(III) pyrimidine-complexes and theoretical studies on the proton affinity of the coordinated ligands. <i>Polyhedron</i> , 2010, 29, 1833-1836. | 1.0 | 3 |
| 4693 | Evaluation of dispersion-corrected density functional theory (B3LYP-DCP) for compounds of biochemical interest. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 29, 178-187. | 1.3 | 19 |
| 4694 | Gas phase infrared spectra and corresponding DFT calculations of β , γ -diphenylpolyenes. <i>Journal of Molecular Spectroscopy</i> , 2010, 259, 11-15. | 0.4 | 4 |
| 4695 | A DFT study on the effect of hydrogen bonding on the reaction of a η^4 -benzoquinone diruthenium complex with acetylene. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 552-557. | 0.8 | 4 |
| 4696 | Structural characterization of triorganotin(IV) complexes with sodium fusidate and DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 1405-1413. | 0.8 | 6 |
| 4697 | DFT study of alkene hydrogenation catalyzed by Rh(acac)(CO) ₂ . <i>Journal of Organometallic Chemistry</i> , 2010, 695, 1576-1582. | 0.8 | 14 |
| 4698 | Theoretical study on ligand exchange reaction mechanisms of iron(IV) complexes with two different group 14 element ligands, Cp(CO)FeH(Et ₃)(E ₂) with (HEt ₃) (E, E ₂ = Si, Ge, Sn). <i>Journal of Organometallic Chemistry</i> , 2010, 695, 1682-1687. | 0.8 | 2 |
| 4699 | DFT study of the mechanism of Cu(I)-catalyzed and uncatalyzed intramolecular cyclopropanation of iodonium ylides. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 2030-2038. | 0.8 | 7 |
| 4700 | Computational study of reaction pathways in the course of interaction of deactivated silylenes with buta-1,3-diene. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 2345-2353. | 0.8 | 7 |
| 4701 | Assignment of the absolute configuration at the sulfur atom of thioridazine metabolites by the analysis of their chiroptical properties: The case of thioridazine 2-sulfoxide. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2010, 52, 796-801. | 1.4 | 10 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4702 | The mechanisms of ROS-photogeneration by berberine, a natural isoquinoline alkaloid. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2010, 99, 154-156. | 1.7 | 12 |
| 4703 | Cis-trans isomerism in cobalt(II) complexes with 3-hydroxypicolinic acid. Structural, DFT and thermal studies. <i>Inorganica Chimica Acta</i> , 2010, 363, 1887-1896. | 1.2 | 12 |
| 4704 | {Ru(NO) ₆ } and {Ru(NO) ₇ } configurations in [Ru(trpy)(tmp)(NO)] ⁿ⁺ (trpy=2,2',6'-terpyridine, tmp=2,2',6'-terpyridine.) <i>Inorganica Chimica Acta</i> , 2010, 363, 2945-2954. | 1.2 | 20 |
| 4705 | Synthesis, characterization and in vitro cytotoxicity studies of platinum(IV) complexes with thiouracil ligands. <i>Inorganica Chimica Acta</i> , 2010, 363, 2452-2460. | 1.2 | 12 |
| 4706 | Ruthenium(II) thiocrown complexes: Synthetic, spectroscopic, electrochemical, DFT, and single crystal X-ray structural studies of [Ru([15]aneS5)Cl](PF ₆). <i>Inorganica Chimica Acta</i> , 2010, 364, 55-60. | 1.2 | 6 |
| 4707 | A model study of effect of M ⁺ =Li ⁺ , Na ⁺ , Be ²⁺ , Mg ²⁺ , and Al ³⁺ ion decoration on hydrogen adsorption of metal-organic framework-5. <i>International Journal of Hydrogen Energy</i> , 2010, 35, 12846-12857. | 3.8 | 59 |
| 4708 | Photodissociation and DFT investigation of V ⁺ (C ₂ H ₄) _n (n=1-3) complexes. <i>International Journal of Mass Spectrometry</i> , 2010, 295, 36-42. | 0.7 | 6 |
| 4709 | Binding energy of d10 transition metals to alkenes by wave function theory and density functional theory. <i>Journal of Molecular Catalysis A</i> , 2010, 324, 80-88. | 4.8 | 50 |
| 4710 | Trans effects in the Heck reaction. A model study. <i>Journal of Molecular Catalysis A</i> , 2010, 328, 108-113. | 4.8 | 18 |
| 4711 | Tautomeric and conformational properties of 1,2-diketones. <i>Journal of Molecular Structure</i> , 2010, 978, 282-293. | 1.8 | 42 |
| 4712 | Structure of 1-methyl-6-oxyquinolinium betaine dihydrate studied by X-ray diffraction, DFT calculations, vibrational and NMR spectra. <i>Journal of Molecular Structure</i> , 2010, 976, 87-96. | 1.8 | 10 |
| 4713 | Spectroscopic studies, molecular structure and hydrogen bonding in hydrates of Gemini betaines. <i>Journal of Molecular Structure</i> , 2010, 973, 163-172. | 1.8 | 12 |
| 4714 | The hydrogen bonding network in the dimer of syn-N-phenyl-N'-sulfinylhydrazine, PhNHNSO. <i>Journal of Molecular Structure</i> , 2010, 979, 101-107. | 1.8 | 7 |
| 4715 | Synthesis, characterization and non-linear optical properties of Tetrakis(dimethylammonium) Bromide Hexabromobismuthate: [(CH ₃) ₂ NH ₂] ⁺ ₄ ·Br ⁻ ₄ ·[BiBr ₆] ³⁻ . <i>Journal of Molecular Structure</i> , 2010, 984, 23-29. | 1.8 | 45 |
| 4716 | Experimental and theoretical studies of the molecular structure of 4-(3-(1H-imidazol-1-yl)propyl)-5-p-tolyl-2H-1,2,4-triazol-3(4H)-one. <i>Journal of Molecular Structure</i> , 2010, 984, 137-145. | 1.8 | 21 |
| 4717 | Structural, spectroscopic and theoretical studies of short OHO hydrogen bonds in 2:1 complexes of 1-methyl-6-oxyquinolinium betaine with mineral acids. <i>Journal of Molecular Structure</i> , 2010, 984, 326-331. | 1.8 | 0 |
| 4718 | Full vs. constrain geometry optimization in the open-closed method in estimating the energy of intramolecular charge-inverted hydrogen bonds. <i>Chemical Physics</i> , 2010, 376, 76-83. | 0.9 | 40 |
| 4719 | Colorimetric and fluorometric sensing of the Lewis acidity of a metal ion by metal-ion complexation of imidazo[1,2-a]pyrazin-3(7H)-ones. <i>Tetrahedron</i> , 2010, 66, 3842-3848. | 1.0 | 13 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4720 | A new bis(pyrenyl)azadiene-based probe for the colorimetric and fluorescent sensing of Cu(II) and Hg(II). <i>Tetrahedron</i> , 2010, 66, 3662-3667. | 1.0 | 76 |
| 4721 | Catalyst electronic polarizability and enantiomeric excess in asymmetric hydrogenation. <i>Tetrahedron</i> , 2010, 66, 4560-4563. | 1.0 | 12 |
| 4722 | The stereochemical assignment of acyclic polyols: a computational study of the NMR data of a library of stereopentad sequences from polyketide natural products. <i>Tetrahedron</i> , 2010, 66, 6437-6444. | 1.0 | 24 |
| 4723 | Asymmetric Mannich reaction catalyzed by N-arylsulfonyl-L-proline amides. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 58-61. | 1.8 | 24 |
| 4724 | Memory and dynamics in Pd-catalyzed allylic alkylation with P,N-ligands. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 1585-1592. | 1.8 | 26 |
| 4725 | Synthesis and properties of bis(pyrazino[2,3- <i>b</i> :4,5- <i>i</i>]imidazole)-fused 1,2,5,6-tetrahydro-1,4,5,8,9,10-hexaazaanthracenes: a new fluorescent nitrogen-rich heterocycle. <i>Tetrahedron Letters</i> , 2010, 51, 1401-1403. | 0.7 | 10 |
| 4726 | Synthesis and fluorescence properties of difluoro[amidopyrazinato-O,N]boron derivatives: a new boron-containing fluorophore. <i>Tetrahedron Letters</i> , 2010, 51, 1613-1615. | 0.7 | 25 |
| 4727 | Selective sensing of Zn(II) ion by a simple anthracene-based tripodal chemosensor. <i>Tetrahedron Letters</i> , 2010, 51, 4995-4999. | 0.7 | 41 |
| 4728 | Theoretical study of the dynamics and thermal mechanisms of the reaction: Dehydration of glycerol to glycidol. <i>Computational and Theoretical Chemistry</i> , 2010, 942, 38-42. | 1.5 | 17 |
| 4729 | A study on the electronic and structural properties of fullerene C ₃₀ and azafullerene C ₁₈ N ₁₂ . <i>Computational and Theoretical Chemistry</i> , 2010, 942, 71-76. | 1.5 | 7 |
| 4730 | Evaluation of density functionals, SCC-DFTB, neglect of diatomic differential overlap (NDDO) models and molecular mechanics methods for prolyl-leucyl-glycinamide (PLG) and structural analogs. <i>Computational and Theoretical Chemistry</i> , 2010, 944, 76-82. | 1.5 | 1 |
| 4731 | Intramolecular charge-inverted hydrogen bond. <i>Computational and Theoretical Chemistry</i> , 2010, 948, 21-24. | 1.5 | 23 |
| 4732 | Cu ²⁺ binding chalcogen-chalcogen bridges: A problematic case for DFT. <i>Computational and Theoretical Chemistry</i> , 2010, 954, 7-15. | 1.5 | 12 |
| 4733 | An insight into microscopic properties of aprotic ionic liquids: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2010, 955, 47-52. | 1.5 | 16 |
| 4734 | van der Waals interactions in sterically crowded disilenes. <i>Computational and Theoretical Chemistry</i> , 2010, 957, 66-71. | 1.5 | 7 |
| 4735 | Electronic isomerization in fullerene: A density functional trial. <i>Computational and Theoretical Chemistry</i> , 2010, 958, 122-132. | 1.5 | 5 |
| 4736 | Conformational analysis of cycloheptanone and cycloheptanethione. <i>Computational and Theoretical Chemistry</i> , 2010, 959, 62-65. | 1.5 | 7 |
| 4737 | Density functional study of the nitrosamine-formic acid and nitrosamine-formamide interactions. <i>Computational and Theoretical Chemistry</i> , 2010, 960, 15-21. | 1.5 | 2 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 4738 | Hydrazine (N ₂ H ₄) adsorption on Ni(100) – Density functional theory investigation. <i>Surface Science</i> , 2010, 604, 245-251. | 0.8 | 48 |
| 4739 | Experimental (FT-IR, FT-RS) and theoretical (DFT) studies of vibrational dynamics and molecular structure of 4-n-pentylphenyl-4- ² -n-octyloxythiobenzoate (8OS5). <i>Vibrational Spectroscopy</i> , 2010, 52, 54-62. | 1.2 | 29 |
| 4740 | DFT, FT-Raman, FT-IR, liquid and solid state NMR studies of 2,6-dimethoxyphenylboronic acid. <i>Vibrational Spectroscopy</i> , 2010, 54, 1-9. | 1.2 | 66 |
| 4741 | Quantum chemical insights into the initiation mechanism of transition metal catalysed polymerisation of isobutene. <i>Applied Catalysis A: General</i> , 2010, 384, 154-164. | 2.2 | 7 |
| 4742 | Mn(II) – A fascinating oxidation catalyst: Mechanistic insight into the catalyzed oxidative degradation of organic dyes by H ₂ O ₂ . <i>Applied Catalysis B: Environmental</i> , 2010, 95, 179-191. | 10.8 | 48 |
| 4743 | The pH effect on black spots in surface finish: Electroless nickel immersion gold. <i>Applied Surface Science</i> , 2010, 257, 56-61. | 3.1 | 31 |
| 4744 | Electrochemical and density functional studies of the catalytic ethylene oxidation on nanostructured Au electrodes. <i>Catalysis Today</i> , 2010, 158, 29-34. | 2.2 | 18 |
| 4745 | Non-quantum-confinement optics in (CdS) _n clusters. <i>Chemical Physics</i> , 2010, 368, 113-120. | 0.9 | 28 |
| 4746 | Monitoring peptide-surface interaction by means of molecular dynamics simulation. <i>Chemical Physics</i> , 2010, 378, 73-81. | 0.9 | 11 |
| 4747 | NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. <i>Computer Physics Communications</i> , 2010, 181, 1477-1489. | 3.0 | 4,740 |
| 4748 | 1-(3-Deoxy-3-fluoro- ² -d-glucopyranosyl) pyrimidine derivatives as inhibitors of glycogen phosphorylase b: Kinetic, crystallographic and modelling studies. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 3413-3425. | 1.4 | 35 |
| 4749 | Search for influence of spatial properties on affinity at α 1-adrenoceptor subtypes for phenylpiperazine derivatives of phenytoin. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 6152-6156. | 1.0 | 18 |
| 4750 | Protic and aprotic solvent effect on molecular properties and g-tensors of o-semiquinones with various aromaticity and heteroatoms: A DFT study. <i>Chemical Physics Letters</i> , 2010, 493, 364-370. | 1.2 | 14 |
| 4751 | Assessment of density functional methods for the study of olefin metathesis catalysed by ruthenium alkylidene complexes. <i>Chemical Physics Letters</i> , 2010, 493, 273-278. | 1.2 | 60 |
| 4752 | EPR spin trapping and DFT studies on structure of active antioxidants in bioglycerol. <i>Chemical Physics Letters</i> , 2010, 497, 135-141. | 1.2 | 14 |
| 4753 | Calculated two-photon electronic transitions in sulfuric acid and its atmospheric relevance. <i>Chemical Physics Letters</i> , 2010, 498, 18-21. | 1.2 | 1 |
| 4754 | Electron affinities of d1 transition metal chloride clusters and onset of super halogen behavior. <i>Chemical Physics Letters</i> , 2010, 498, 56-62. | 1.2 | 19 |
| 4755 | Theoretical investigation for the reaction of N ₂ O with CO catalyzed by MO ⁺ (M=Ru, Os). <i>Chemical Physics Letters</i> , 2010, 498, 245-252. | 1.2 | 5 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4756 | Divide-and-conquer self-consistent field calculation for open-shell systems: Implementation and application. <i>Chemical Physics Letters</i> , 2010, 500, 172-177. | 1.2 | 43 |
| 4757 | From the Lithium ²⁺ anilide ²⁻ fluoro ^{1,3} diaz ²⁺ sila ²⁻ cyclopentene ⁺ GaCl ₃ Adduct to 1,4-Triaza ⁵⁺ Gallium ⁷⁺ sila ³⁻ cyclo ³ heptene ⁺ Experimental and Quantum ⁺ chemical Results. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2010, 636, 1527-1532. | | |
| 4758 | [(BeCl ₂) ₂ (18-Krone-6)] und sein Hydrolyseprodukt [{Be ₃ (¹ / ₄ -OH) ₃ (H ₂ O) ₆ -(18-Krone-6)]Cl ₃ ·3H ₂ O: Kristallstrukturen und DFT-Rechnungen. [(BeCl ₂) ₂ (18-Crown-6)] and its Product of Hydrolysis [{Be ₃ (¹ / ₄ -OH) ₃ (H ₂ O) ₆ -(18-Crown-6)]Cl ₃ ·3H ₂ O: Crystal Structures and DFT C. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2010, 636, 2364-2371. | 0.6 | 23 |
| 4759 | Synthesis and properties of new aromatic polyisophthalamides with adamantylamide pendent groups. <i>Journal of Polymer Science Part A</i> , 2010, 48, 1743-1751. | 2.5 | 45 |
| 4760 | Density functional study on the effect of substituent group for the monomer of donor ⁺ acceptor copolymer. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2010, 48, 2099-2107. | 2.4 | 15 |
| 4761 | Influence of imidazolium ⁺ based ionic liquids on the performance of ionic polymer conductor network composite actuators. <i>Polymer International</i> , 2010, 59, 321-328. | 1.6 | 67 |
| 4762 | Systematic conformational search analysis of the SRR and RRR epimers of 7 ⁺ hydroxymatairesinol. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 141-147. | 0.9 | 6 |
| 4763 | Computational modeling of human paraoxonase 1: preparation of protein models, binding studies, and mechanistic insights. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 357-369. | 0.9 | 19 |
| 4764 | Theoretical study of structural and optical properties of small silver and gold clusters at defect centers of MgO. <i>Physica Status Solidi (B): Basic Research</i> , 2010, 247, 1099-1108. | 0.7 | 6 |
| 4765 | CASSCF/CASPT2 analysis of the fragmentation of H ₂ on a Pd ₄ cluster. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 558-562. | 1.0 | 19 |
| 4766 | On the performance of eleven DFT functionals in the description of the vibrational properties of aluminosilicates. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 406-415. | 1.0 | 121 |
| 4767 | Theoretical studies on the electronic structures and spectroscopic properties of a series of novel Ni ²⁺ Ci ²⁺ N ³⁻ coordinating Pt(II) complexes. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 1605-1614. | 1.0 | 1 |
| 4768 | Elongation cutoff technique at Kohn ⁺ Sham level of theory. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2130-2139. | 1.0 | 19 |
| 4769 | Performance of 12 DFT functionals in the study of crystal systems: Al ₂ SiO ₅ orthosilicates and Al hydroxides as a case study. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2260-2273. | 1.0 | 42 |
| 4770 | Theoretical study of NMR chemical shift induced by H/D isotope effect. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2989-2995. | 1.0 | 7 |
| 4771 | Synthesis, characterization, and studies on DNA binding of the complex Fe(Sal ₂ dienNO ₃ ·H ₂ O). <i>Biochemistry (Moscow)</i> , 2010, 75, 505-512. | 0.7 | 5 |
| 4773 | 2. The Minnesota Density Functionals and their Applications to Problems in Mineralogy and Geochemistry. , 2010, , 19-38. | | 4 |
| 4774 | Anthracene appended pyridinium amide ⁺ urea conjugate in selective fluorometric sensing of L- <i>N</i> - <i>l</i> acetylvaline salt. <i>Beilstein Journal of Organic Chemistry</i> , 2010, 6, 1211-1218. | 1.3 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4775 | The 15 ⁺ 20 ⁺ 4 ⁺ PAH emission features: probes of individual PAHs?. <i>Astronomy and Astrophysics</i> , 2010, 511, A32. | 2.1 | 74 |
| 4776 | TORSIONAL POTENTIALS AND FULL-DIMENSIONAL SIMULATION OF ELECTRONIC ABSORPTION SPECTRA OF <i>p</i> -PHENYLENEVINYLENE OLIGOMERS USING SEMIEMPIRICAL HAMILTONIANS. <i>Journal of Theoretical and Computational Chemistry</i> , 2010, 09, 249-263. | 1.8 | 13 |
| 4777 | The Aromatic Amino Acid Hydroxylase Mechanism: A Perspective From Computational Chemistry. <i>Advances in Inorganic Chemistry</i> , 2010, , 437-500. | 0.4 | 11 |
| 4778 | Structural analysis of the antimalarial drug halofantrine by means of Raman spectroscopy and density functional theory calculations. <i>Journal of Biomedical Optics</i> , 2010, 15, 041516. | 1.4 | 47 |
| 4779 | Comparison between Investigational IR and Crystallographic Data with Computational Chemistry Tools as Validation of the Methods. <i>Advances in Physical Chemistry</i> , 2010, 2010, 1-5. | 2.0 | 3 |
| 4780 | On the Importance of Clar Structures of Polybenzenoid Hydrocarbons as Revealed by the π -Contribution to the Electron Localization Function. <i>Symmetry</i> , 2010, 2, 1653-1682. | 1.1 | 41 |
| 4781 | Evaporation temperature-tuned physical vapor deposition growth engineering of one-dimensional non-Fermi liquid tetrathiofulvalene tetracyanoquinodimethane thin films. <i>Applied Physics Letters</i> , 2010, 97, 111906. | 1.5 | 10 |
| 4782 | Density functional theory, restricted Hartree-Fock simulations and vibrational spectroscopic studies of nicorandil. <i>Molecular Simulation</i> , 2010, 36, 425-433. | 0.9 | 27 |
| 4783 | XYG3s: Speedup of the XYG3 fifth-rung density functional with scaling-all-correlation method. <i>Journal of Chemical Physics</i> , 2010, 132, 194105. | 1.2 | 40 |
| 4784 | Tests of the RPBE, revPBE, $\ddot{\text{I}}$,-HCTHhyb, $\ddot{\text{I}}$ ₈₆ B97X-D, and MOHLYP density functional approximations and 29 others against representative databases for diverse bond energies and barrier heights in catalysis. <i>Journal of Chemical Physics</i> , 2010, 132, 164117. | 1.2 | 206 |
| 4785 | Electronic structure of single-layered undoped cuprates from hybrid density functional theory. <i>Physical Review B</i> , 2010, 81, . | 1.1 | 34 |
| 4786 | Electronic structures of [n]-cyclacenes (n = 6-12) and short, hydrogen-capped, carbon nanotubes. <i>Faraday Discussions</i> , 0, 145, 507-521. | 1.6 | 39 |
| 4787 | Active-space completely-renormalized equation-of-motion coupled-cluster formalism: Excited-state studies of green fluorescent protein, free-base porphyrin, and oligoporphyrin dimer. <i>Journal of Chemical Physics</i> , 2010, 132, 154103. | 1.2 | 59 |
| 4788 | Applications of QM/MM in inorganic chemistry. <i>Spectroscopic Properties of Inorganic and Organometallic Compounds</i> , 0, , 87-110. | 0.4 | 1 |
| 4789 | X-ray structure analysis and DFT study of a chiral (salen)Mn(III) complex toward understanding of inversion of enantioselection in epoxidation catalysts. <i>Journal of Coordination Chemistry</i> , 2010, 63, 2868-2878. | 0.8 | 7 |
| 4790 | Synthesis, molecular and electronic structure of half-sandwich ruthenium(II) complex with 2-(2-pyridyl)-4-methylthiazole-5-carboxylic acid. <i>Journal of Coordination Chemistry</i> , 2010, 63, 2268-2277. | 0.8 | 2 |
| 4791 | A first principles study of fluorescence quenching in rhodamine B dimers: how can quenching occur in dimeric species?. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 11238. | 1.3 | 103 |
| 4792 | Effects of Electronic and Lattice Polarization on the Band Structure of Delafossite Transparent Conductive Oxides. <i>Physical Review Letters</i> , 2010, 104, 136401. | 2.9 | 88 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4793 | Extension of energy density analysis to periodic-boundary-condition calculations with plane-wave basis functions. <i>Physical Review B</i> , 2010, 81, . | 1.1 | 2 |
| 4794 | The structure, stability, and reactivity of oxalato-monoperoxovanadium(V) in solution. <i>Journal of Coordination Chemistry</i> , 2010, 63, 3268-3278. | 0.8 | 3 |
| 4795 | NMR and theoretical study on the interaction between diperoxovanadate and 3-picoline derivatives. <i>Journal of Coordination Chemistry</i> , 2010, 63, 1555-1562. | 0.8 | 5 |
| 4796 | Electronic hyperpolarizability calculation without the periodic images error for a large nonlinear molecule. <i>Physical Review B</i> , 2010, 81, . | 1.1 | 4 |
| 4797 | Peierls instability in carbon nanotubes: A first-principles study. <i>Physical Review B</i> , 2010, 82, . | 1.1 | 25 |
| 4798 | Systematic investigation of a family of gradient-dependent functionals for solids. <i>Physical Review B</i> , 2010, 81, . | 1.1 | 36 |
| 4799 | Density functional study of CO and NO adsorption on Ni-doped MgO(100). <i>Journal of Chemical Physics</i> , 2010, 132, 104701. | 1.2 | 52 |
| 4800 | Oxidation of pinacyanol chloride by H ₂ O ₂ catalyzed by Fe(III) complexed to tetraamidomacrocyclic ligand: unusual kinetics and product identification. <i>Journal of Coordination Chemistry</i> , 2010, 63, 2605-2618. | 0.8 | 17 |
| 4801 | THE NASA AMES POLYCYCLIC AROMATIC HYDROCARBON INFRARED SPECTROSCOPIC DATABASE: THE COMPUTED SPECTRA. <i>Astrophysical Journal, Supplement Series</i> , 2010, 189, 341-351. | 3.0 | 163 |
| 4802 | THEORETICAL STUDY ON THE H ₂ ACTIVATION BY PtO ₂ AND PtO_{2}^{+} IN THE GAS PHASE. <i>Journal of Theoretical and Computational Chemistry</i> , 2010, 09, 963-974. | 1.8 | 2 |
| 4803 | Configurational Properties of N,N-Dimethyl-1,3-Diazacyclohexane and Its Analogues Containing P and As Atoms: A Hybrid-DFT Study and NBO Interpretation. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2010, 186, 44-57. | 0.8 | 2 |
| 4804 | Basis set dependence of the doubly hybrid XYG3 functional. <i>Journal of Chemical Physics</i> , 2010, 133, 104105. | 1.2 | 41 |
| 4805 | B3LYP Study on Reduction Mechanisms from to at the Catalytic Sites of Fully Reduced and Mixed-Valence Bovine Cytochrome Oxidases. <i>Bioinorganic Chemistry and Applications</i> , 2010, 2010, 1-18. | 1.8 | 6 |
| 4806 | Insight into the Strong Antioxidant Activity of Deinoxanthin, a Unique Carotenoid in <i>Deinococcus Radiodurans</i> . <i>International Journal of Molecular Sciences</i> , 2010, 11, 4506-4510. | 1.8 | 29 |
| 4807 | The Variety of Carbon-Metal Bonds inside Cu-ZSM-5 Zeolites: A Density Functional Theory Study. <i>Materials</i> , 2010, 3, 2516-2535. | 1.3 | 15 |
| 4808 | Reductive half-reaction of aldehyde oxidoreductase toward acetaldehyde: Ab initio and free energy quantum mechanical/molecular mechanical calculations. <i>Journal of Chemical Physics</i> , 2010, 132, 035101. | 1.2 | 33 |
| 4809 | Localized Hartree product treatment of multiple protons in the nuclear-electronic orbital framework. <i>Journal of Chemical Physics</i> , 2010, 132, 084110. | 1.2 | 21 |
| 4810 | Relativistic four- and two-component calculations of parity violation effects in chiral tungsten molecules of the form NWXYZ (X, Y, Z=H, F, Cl, Br, or I). <i>Journal of Chemical Physics</i> , 2010, 132, 234310. | 1.2 | 14 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4811 | Synthesis and formation mechanism of hydrogenated boron clusters B ₁₂ H _n with controlled hydrogen content. <i>Journal of Chemical Physics</i> , 2010, 133, 074305. | 1.2 | 17 |
| 4812 | The axial methionine ligand may control the redox reorganizations in the active site of blue copper proteins. <i>Journal of Chemical Physics</i> , 2010, 133, 175101. | 1.2 | 12 |
| 4813 | Roles of radical characters of pristine and nitrogen-substituted hydrographene in dioxygen bindings. <i>Journal of Chemical Physics</i> , 2010, 133, 174703. | 1.2 | 6 |
| 4814 | Charge transport in columnar mesophases of carbazole macrocycles. <i>Journal of Chemical Physics</i> , 2010, 133, 134901. | 1.2 | 16 |
| 4815 | Prediction of Excitation Energies for Conjugated Oligomers and Polymers from Time-Dependent Density Functional Theory. <i>Materials</i> , 2010, 3, 3430-3467. | 1.3 | 3 |
| 4816 | THE FAR-INFRARED SPECTROSCOPY OF VERY LARGE NEUTRAL POLYCYCLIC AROMATIC HYDROCARBONS. <i>Astrophysical Journal</i> , 2010, 709, 42-52. | 1.6 | 28 |
| 4817 | Theoretical study of the structural and electronic properties of the Fe(C ₆ H ₆) _m , n = 2; m = 2 complexes. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7545. | 1.3 | 18 |
| 4818 | R-matrix calculation of low-energy electron collisions with phosphoric acid. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2010, 43, 235203. | 0.6 | 14 |
| 4819 | A multiscale study of electronic structure and quantum transport in C ₆ N ₂ H ₆ -based graphene quantum dots. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 095504. | 0.7 | 13 |
| 4820 | Molecular applications of analytical gradient approach for the improved virtual orbital-complete active space configuration interaction method. <i>Journal of Chemical Physics</i> , 2010, 132, 034105. | 1.2 | 12 |
| 4821 | Rung 3.5 density functionals. <i>Journal of Chemical Physics</i> , 2010, 133, 104103. | 1.2 | 36 |
| 4822 | Ab initio studies of ultrafast x-ray scattering of the photodissociation of iodine. <i>Journal of Chemical Physics</i> , 2010, 133, 124309. | 1.2 | 19 |
| 4823 | A density-functional study of the adsorption of methane-thiol on the (111) surfaces of the Ni-group metals: II. Vibrational spectroscopy. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 265006. | 0.7 | 68 |
| 4824 | Electronic transport calculations for the conductance of Pt-1,4-phenylene diisocyanide-Pt molecular junctions. <i>Nanotechnology</i> , 2010, 21, 155203. | 1.3 | 9 |
| 4825 | A density functional study of the adsorption of methane-thiol on the (111) surfaces of the Ni-group metals: I. Molecular and dissociative adsorption. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 265005. | 0.7 | 19 |
| 4826 | Hydrogen-Bonding-Promoted Oxidative Addition and Regioselective Arylation of Olefins with Aryl Chlorides. <i>Journal of the American Chemical Society</i> , 2010, 132, 16689-16699. | 6.6 | 104 |
| 4827 | Metal-Metal and Metal-Ligand Bonding at a QTAIM Catastrophe: A Combined Experimental and Theoretical Charge Density Study on the Alkylidyne Cluster Fe ₃ (1/4-H)(1/4-COMe)(CO) ₁₀ . <i>Journal of Physical Chemistry A</i> , 2010, 114, 13418-13433. | 1.1 | 91 |
| 4828 | Sorting Out the Relative Contributions of Electrostatic Polarization, Dispersion, and Hydrogen Bonding to Solvatochromic Shifts on Vertical Electronic Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2829-2844. | 2.3 | 45 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4829 | Computational Studies of the Interaction between Ruthenium Dyes and $X\hat{\sigma}^{\bullet}$ and $X2\hat{\sigma}^{\bullet}$, X = Br, I, At. Implications for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2010, 114, 15165-15173. | 1.5 | 25 |
| 4830 | DFT Studies on the Carboxylation of Arylboronate Esters with CO_2 Catalyzed by Copper(I) Complexes. <i>Organometallics</i> , 2010, 29, 917-927. | 1.1 | 116 |
| 4831 | Vibrational Circular Dichroism and IR Absorption Spectra of Amino Acids: A Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 3591-3601. | 1.1 | 17 |
| 4832 | Electric field induced activation of H_2 "Can DFT do the job?". <i>Chemical Communications</i> , 2010, 46, 7942. | 2.2 | 106 |
| 4833 | In situ alkylation of N-heterocycles in organic templated cuprous halides. <i>Dalton Transactions</i> , 2010, 39, 2701. | 1.6 | 49 |
| 4834 | Redox-Active Ligands Facilitate Bimetallic O_2 Homolysis at Five-Coordinate Oxorhenium(V) Centers. <i>Journal of the American Chemical Society</i> , 2010, 132, 3879-3892. | 6.6 | 98 |
| 4835 | Design of Energetic Ionic Liquids. , 2010, , . | | 1 |
| 4836 | Some Geometric and Electronic Structural Effects of Perfluorinating Propionyl Chloride. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8009-8015. | 1.1 | 27 |
| 4837 | Effect of chemical change on TDDFT accuracy: orbital overlap perspective of the hydrogenation of retinal. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2816. | 1.3 | 37 |
| 4838 | Characterization of Nucleobase Analogue FRET Acceptor tC_{nitro} . <i>Journal of Physical Chemistry B</i> , 2010, 114, 1050-1056. | 1.2 | 39 |
| 4839 | Understanding the NMR chemical shifts for 6-halopurines: role of structure, solvent and relativistic effects. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5126. | 1.3 | 44 |
| 4840 | Novel Acyclic Diaminocarbene Ligands with Increased Steric Demand and Their Application in Gold Catalysis. <i>Organic Letters</i> , 2010, 12, 4860-4863. | 2.4 | 70 |
| 4841 | Effects of the Metal Center and Substituting Groups on the Linear and Nonlinear Optical Properties of Substituted Styryl-Bipyridine Metal(II) Dichloride Complexes: DFT and TDDFT Computational Investigations and Harmonic Light Scattering Measurements. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5429-5438. | 1.1 | 28 |
| 4842 | Mechanistic Comparison of Acid- and Gold(I)-Catalyzed Nucleophilic Addition Reactions to Olefins. <i>Organometallics</i> , 2010, 29, 5919-5926. | 1.1 | 46 |
| 4843 | Modelling nano-clusters and nucleation. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 786-811. | 1.3 | 174 |
| 4844 | Energy landscape of silicon systems and its description by force fields, tight binding schemes, density functional methods, and quantum Monte Carlo methods. <i>Physical Review B</i> , 2010, 81, . | 1.1 | 31 |
| 4845 | Copper(II) and Nickel(II) Complexes of \hat{I}^2 -Aminoketoxime Ligand: Syntheses, Crystal Structures, Magnetism, and Nickel(II) Templated Coupling of Oxime with Nitrile. <i>Inorganic Chemistry</i> , 2010, 49, 541-551. | 1.9 | 29 |
| 4846 | Accurate calculation and modeling of the adiabatic connection in density functional theory. <i>Journal of Chemical Physics</i> , 2010, 132, 164115. | 1.2 | 86 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4847 | Describing Both Dispersion Interactions and Electronic Structure Using Density Functional Theory: The Case of Metal ⁺ Phthalocyanine Dimers. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 81-90. | 2.3 | 109 |
| 4848 | Quantum chemical dissection of the classic terpinyl/pinyl/bornyl/camphyl cation conundrum—the role of pyrophosphate in manipulating pathways to monoterpenes. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 4589. | 1.5 | 73 |
| 4849 | A general measure of conjugation in biphenyls and their radical cations. <i>Canadian Journal of Chemistry</i> , 2010, 88, 1175-1185. | 0.6 | 17 |
| 4850 | Unsymmetric Ru(II) Complexes with <i>N</i> -Heterocyclic Carbene and/or Terpyridine Ligands: Synthesis, Characterization, Ground- and Excited-State Electronic Structures and Their Application for DSSC Sensitizers. <i>Inorganic Chemistry</i> , 2010, 49, 7340-7352. | 1.9 | 93 |
| 4851 | Factors Dictating Carbene Formation at (PNP)Ir. <i>Organometallics</i> , 2010, 29, 4239-4250. | 1.1 | 16 |
| 4852 | A DFT exploration of the organization of thiols on Au(111): a route to self-assembled monolayer of magnetic molecules. <i>Journal of Materials Chemistry</i> , 2010, 20, 10747. | 6.7 | 24 |
| 4853 | Structure and Spectroscopic Properties of Iron Oxides with the High Content of Oxygen: FeO _n and FeO _n ⁺ (<i>n</i> = 5–12). <i>Journal of Physical Chemistry A</i> , 2010, 114, 9014-9021. | 1.1 | 36 |
| 4854 | ALD Growth Characteristics of ZnS Films Deposited from Organozinc and Hydrogen Sulfide Precursors. <i>Langmuir</i> , 2010, 26, 11899-11906. | 1.6 | 37 |
| 4855 | Assessment of TD-DFT methods and of various spin scaled CIS(D) and CC2 versions for the treatment of low-lying valence excitations of large organic dyes. <i>Journal of Chemical Physics</i> , 2010, 132, . | 1.2 | 313 |
| 4856 | Computing Second-Order Functional Derivatives with Respect to the External Potential. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3671-3680. | 2.3 | 34 |
| 4857 | Computational Study of Molecules with High Intrinsic Hyperpolarizabilities. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10676-10683. | 1.1 | 17 |
| 4858 | Structure and energetics of imogolite: a quantum mechanical ab initio study with B3LYP hybrid functional. <i>Journal of Materials Chemistry</i> , 2010, 20, 10417. | 6.7 | 41 |
| 4859 | Two-Electron Redox Energetics in Ligand-Bridged Dinuclear Molybdenum and Tungsten Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 4611-4619. | 1.9 | 24 |
| 4860 | Novel Layer-by-Layer Interfacial [Ni(salen)] ⁺ Polyelectrolyte Hybrid Films. <i>Langmuir</i> , 2010, 26, 10842-10853. | 1.6 | 22 |
| 4861 | Vibrational Circular Dichroism Spectroscopy of Chiral Molecules. <i>Topics in Current Chemistry</i> , 2010, 298, 189-236. | 4.0 | 65 |
| 4862 | A Test to Evaluate the Performance of Aromaticity Descriptors in All-Metal and Semimetal Clusters. An Appraisal of Electronic and Magnetic Indicators of Aromaticity. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1118-1130. | 2.3 | 84 |
| 4863 | Thiocyanation of closo-Dodecaborate B ₁₂ H ₁₂ ⁺ . A Novel Synthetic Route and Theoretical Elucidation of the Reaction Mechanism. <i>Inorganic Chemistry</i> , 2010, 49, 5040-5048. | 1.9 | 13 |
| 4864 | Theory of Excited State Decays and Optical Spectra: Application to Polyatomic Molecules. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7817-7831. | 1.1 | 363 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4865 | Cyclooctatetraene in metal complexesâ€”planar does not mean aromatic. <i>New Journal of Chemistry</i> , 2010, 34, 1855. | 1.4 | 17 |
| 4866 | The vibrational behavior of silica clusters at the glass transition: Ab initio calculations and thermodynamic implications. <i>Journal of Chemical Physics</i> , 2010, 133, 104508. | 1.2 | 18 |
| 4867 | Indolyne Experimental and Computational Studies: Synthetic Applications and Origins of Selectivities of Nucleophilic Additions. <i>Journal of the American Chemical Society</i> , 2010, 132, 17933-17944. | 6.6 | 215 |
| 4868 | Absorption Spectra of Riboflavinâ€”A Difficult Case for Computational Chemistry. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10234-10242. | 1.1 | 25 |
| 4869 | Using Nonempirical Semilocal Density Functionals and Empirical Dispersion Corrections to Model Dative Bonding in Substituted Boranes. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1825-1833. | 2.3 | 22 |
| 4870 | The fragment spin difference scheme for triplet-triplet energy transfer coupling. <i>Journal of Chemical Physics</i> , 2010, 133, 074105. | 1.2 | 58 |
| 4871 | Global Hybrid Functionals: A Look at the Engine under the Hood. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3688-3703. | 2.3 | 87 |
| 4872 | One-dimensional order in liquid crystals by combining H | 0.8 | 11 |
| 4873 | On the Reactivity of Rhodium(I) Complexes with P -Coordinated P -Phosphino-Functionalized Propyl Phenyl Sulfide Ligands: Routes to Cyclic Rhodium Complexes with C , P - and P , S -Coordinated Ligands as Well as Bis(diphenylphosphino)methanide Ligands. <i>Organometallics</i> , 2010, 29, 6749-6762. | 1.1 | 6 |
| 4874 | Half-Sandwich Iridium Complexes for Homogeneous Water-Oxidation Catalysis. <i>Journal of the American Chemical Society</i> , 2010, 132, 16017-16029. | 6.6 | 507 |
| 4875 | Theoretical Investigation of Solvent Effects on Glycosylation Reactions: Stereoselectivity Controlled by Preferential Conformations of the Intermediate Oxocarbenium-Counterion Complex. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1783-1797. | 2.3 | 137 |
| 4876 | Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2872-2887. | 2.3 | 1,183 |
| 4877 | Toward a General Formulation of Dispersion Effects for Solvation Continuum Models. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3358-3364. | 2.3 | 35 |
| 4878 | A General Database for Main Group Thermochemistry, Kinetics, and Noncovalent Interactions $\hat{\sim}$ Assessment of Common and Reparameterized (meta -)GGA Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 107-126. | 2.3 | 389 |
| 4879 | Mechanism of Water Oxidation by Single-Site Ruthenium Complex Catalysts. <i>Journal of the American Chemical Society</i> , 2010, 132, 1545-1557. | 6.6 | 443 |
| 4880 | Systematic Study of Modifications to Ruthenium(II) Polypyridine Dyads for Electron Injection Enhancement. <i>Inorganic Chemistry</i> , 2010, 49, 2975-2982. | 1.9 | 31 |
| 4881 | Range-separated local hybrids. <i>Journal of Chemical Physics</i> , 2010, 132, 224106. | 1.2 | 41 |
| 4882 | DFT studies on catalytic properties of isolated and carbon nanotube supported Pd ₉ cluster : Part II. Hydro-isomerization of butene isomers. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1323-1330. | 1.3 | 21 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4883 | Effects of London dispersion on the isomerization reactions of large organic molecules: a density functional benchmark study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6940. | 1.3 | 123 |
| 4884 | Modulation of the luminescence quantum efficiency for blue luminophor {Al(salophen)} ⁺ by ester-substituents. <i>Dalton Transactions</i> , 2010, 39, 2070. | 1.6 | 39 |
| 4885 | Hybrid functionals within the all-electron FLAPW method: Implementation and applications of PBE0. <i>Physical Review B</i> , 2010, 81, . | 1.1 | 48 |
| 4886 | Computational Study of Silica-Supported Transition Metal Fragments for Kubas-type Hydrogen Storage. <i>Journal of the American Chemical Society</i> , 2010, 132, 17296-17305. | 6.6 | 30 |
| 4887 | Effective Fragment Molecular Orbital Method: A Merger of the Effective Fragment Potential and Fragment Molecular Orbital Methods ^{â€} . <i>Journal of Physical Chemistry A</i> , 2010, 114, 8705-8712. | 1.1 | 80 |
| 4888 | A density functional theory approach to noncovalent interactions via interacting monomer densities. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 14686. | 1.3 | 9 |
| 4889 | Designing of Disubstituted Derivatives of mer-Alq3: Quantum Theoretical Study. <i>Australian Journal of Chemistry</i> , 2010, 63, 1283. | 0.5 | 11 |
| 4890 | On the Electronic and Structural Properties of Tri-Niobium Oxide Clusters Nb ₃ O _n ^{â€} (n = 3-8): Photoelectron Spectroscopy and Density Functional Calculations. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5958-5966. | 1.1 | 45 |
| 4891 | On the Assessment of Some New Meta-Hybrid and Generalized Gradient Approximation Functionals for Calculations of Anharmonic Vibrational Frequency Shifts in Hydrogen-Bonded Dimers. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4354-4363. | 1.1 | 9 |
| 4892 | The Histidine Effect. Electron Transfer and Capture Cause Different Dissociations and Rearrangements of Histidine Peptide Cation-Radicals. <i>Journal of the American Chemical Society</i> , 2010, 132, 10728-10740. | 6.6 | 55 |
| 4893 | Computational Strategies for Reactions of Aggregated and Solvated Organolithium Carbenoids. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8423-8433. | 1.1 | 28 |
| 4894 | Theoretical Study of the O ₂ Interaction with a Tetrahedral Al ₄ Cluster. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11746-11750. | 1.1 | 19 |
| 4895 | Computational Study of the One- and Two-Photon Absorption and Circular Dichroism of (scp)-Tryptophan. <i>Journal of Physical Chemistry B</i> , 2010, 114, 6500-6512. | 1.2 | 45 |
| 4896 | Theoretical Study on Activation and Protonation of Dinitrogen on Cubane-Type M ₃ S ₄ Clusters (M = V, Cr, Mn, Fe, Co, Ni, Cu, Mo, Ru, and W). <i>Inorganic Chemistry</i> , 2010, 49, 2464-2470. | 1.9 | 13 |
| 4897 | Nonlinear Optical Effects Induced by Nanoparticles in Symmetric Molecules. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20870-20876. | 1.5 | 15 |
| 4898 | Structure and Stereodynamics of Aryldiimino Derivatives. <i>Journal of Organic Chemistry</i> , 2010, 75, 2572-2577. | 1.7 | 2 |
| 4899 | Intramolecular Catalysis of Phosphodiester Hydrolysis by Two Imidazoles. <i>Journal of the American Chemical Society</i> , 2010, 132, 8513-8523. | 6.6 | 45 |
| 4900 | Mechanism and Regioselectivity of the Osmium-Catalyzed Aminohydroxylation of Olefins. <i>Journal of Organic Chemistry</i> , 2010, 75, 1491-1497. | 1.7 | 16 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4901 | Synthesis and Structural and Computational Studies of a Conformationally Locked (η^1 -Perfluoroalkylidene)(η^2 -alkene) Transition Metal Complex: $\text{Ir}(\text{Cp}^*)(\text{CFCF}_3)(\text{C}_2\text{H}_4)$. <i>Organometallics</i> , 2010, 29, 1942-1947. | 1.1 | 23 |
| 4902 | Determination of the Photolysis Products of [FeFe]Hydrogenase Enzyme Model Systems using Ultrafast Multidimensional Infrared Spectroscopy. <i>Inorganic Chemistry</i> , 2010, 49, 9563-9573. | 1.9 | 47 |
| 4903 | Thermal Decomposition and Spectroscopic Studies of Preheated Ammonia Borane. <i>Journal of Physical Chemistry C</i> , 2010, 114, 19529-19534. | 1.5 | 40 |
| 4904 | Tunable Phosphorescent NIR Oxygen Indicators Based on Mixed Benzo- and Naphthoporphyrin Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 9333-9342. | 1.9 | 63 |
| 4905 | Assessment of DFT and DFT-D for Potential Energy Surfaces of Rare Gas Trimers: Implementation and Analysis of Functionals and Extrapolation Procedures. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1951-1965. | 2.3 | 8 |
| 4906 | Electronic Structure of a Paramagnetic $\{\text{MNO}\}_6$ Complex: MnNO 5,5-Tropocoronand. <i>Inorganic Chemistry</i> , 2010, 49, 2701-2705. | 1.9 | 8 |
| 4907 | Mechanism of the Aminolysis of Fischer Alkoxy and Thiocarbene Complexes: A DFT Study. <i>Journal of Organic Chemistry</i> , 2010, 75, 5821-5836. | 1.7 | 19 |
| 4908 | Theoretical Study of the Low-Lying States of $\text{Fe}_2(\text{C}_6\text{H}_6)_3$. <i>Journal of Physical Chemistry A</i> , 2010, 114, 13303-13312. | 1.1 | 4 |
| 4909 | Diffusion of Atomic Oxygen on the Si(100) Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12649-12658. | 1.5 | 18 |
| 4910 | DFT Study on the Mechanism of Amides to Aldehydes Using $\text{Cp}_2\text{Zr}(\text{H})\text{Cl}$. <i>Organometallics</i> , 2010, 29, 42-51. | 1.1 | 22 |
| 4911 | Magnetic Exchange Couplings with Range-Separated Hybrid Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1894-1899. | 2.3 | 53 |
| 4912 | Experimental and Computational Thermodynamic Study of Three Monofluoronitrobenzene Isomers. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7909-7919. | 1.2 | 21 |
| 4913 | Theoretical Studies of $\text{An}_{11}\text{C}_8\text{H}_8$ (An) Tj ETQq_0 0 0 rgBT /Overlock Chemistry, 2010, 49, 6545-6551. | 1.9 | 34 |
| 4914 | Computational Investigation of Reactive to Nonreactive Capture of Carbon Dioxide by Oxygen-Containing Lewis Bases. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11761-11767. | 1.1 | 51 |
| 4915 | Calculation of Magnetic Couplings with Double-Hybrid Density Functionals. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 1201-1204. | 2.1 | 27 |
| 4916 | Energetics and Structural Elucidation of Mechanisms for Gas Phase H/D Exchange of Protonated Peptides. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11953-11963. | 1.1 | 9 |
| 4917 | Revealing the Magnetostructural Dynamics of [2Fe-2S] Ferredoxins from Reduced-Dimensionality Analysis of Antiferromagnetic Exchange Coupling Fluctuations. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11612-11619. | 1.2 | 14 |
| 4918 | Structures and Energetics of Unimolecular Thermal Degradation of Isopropyl Butanoate as a Model Biofuel: Density Functional Theory and Ab Initio Studies. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7996-8002. | 1.1 | 14 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4919 | Density Functional Theory Calculations on Ruthenium(IV) Bis(amido) Porphyrins: Search for a Broader Perspective of Heme Protein Compound II Intermediates. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15380-15388. | 1.2 | 10 |
| 4920 | Calculation of Dramatic Differences in the Activation Energy of Phenyl Migratory Insertion in the Isomers of [Rh(PMe ₃) ₂ Cl(CO)(Ph)H]: Important Effects from Both the Ligand trans to Ph and the Ligand trans to CO. <i>Inorganic Chemistry</i> , 2010, 49, 9162-9168. | 1.9 | 8 |
| 4921 | Intramolecular Hydrogen Bond-Controlled Prolyl Amide Isomerization in Glucosyl 3(<i>S</i>)-Hydroxy-5-hydroxymethylproline Hybrids: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11594-11602. | 1.2 | 7 |
| 4922 | Conformational Preferences of β^2 -Carotene in the Confined Spaces inside Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12139-12144. | 1.5 | 13 |
| 4923 | Cyanide-Bridged Fe(III)-Mn(III) Bimetallic Systems Assembled from the fac-Fe Tricyanide and Mn Schiff bases: Structures, Magnetic Properties, and Density Functional Theory Calculations. <i>Inorganic Chemistry</i> , 2010, 49, 4632-4642. | 1.9 | 44 |
| 4924 | Molecular Mechanisms of Additive Fortification in Model Epoxy Resins: A Solid State NMR Study. <i>Macromolecules</i> , 2010, 43, 7200-7211. | 2.2 | 9 |
| 4925 | Iridium Compounds with β -P,P,Si (biPSi) Pincer Ligands: Favoring Reactive Structures in Unsaturated Complexes. <i>Journal of the American Chemical Society</i> , 2010, 132, 9111-9121. | 6.6 | 61 |
| 4926 | C \equiv C Triple Bond Activation by Heterocyclic Aluminum Phosphinides. <i>Organometallics</i> , 2010, 29, 1323-1330. | 1.1 | 37 |
| 4927 | Copper(I) Olefin Complexes: The Effect of the Trispyrazolylborate Ancillary Ligand in Structure and Reactivity. <i>Organometallics</i> , 2010, 29, 3481-3489. | 1.1 | 32 |
| 4928 | Splitting CO ₂ with Electric Fields: A Computational Investigation. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 3256-3260. | 2.1 | 34 |
| 4929 | Conformational Sampling of Macrocyclic Alkenes Using a Kennard Stone-Based Algorithm. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6879-6887. | 1.1 | 17 |
| 4930 | Density Functional Theory and Isodesmic Reaction Based Prediction of Four Stepwise Protonation Constants, as $\log K_{aH}(\text{pH})$, for Nitrilotriacetic Acid. The Importance of a Kind and Protonated Form of a Reference Molecule Used. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1868-1878. | 1.1 | 19 |
| 4931 | Lactones and Quinones from the Tubers of <i>Sinningia aggregata</i> . <i>Journal of Natural Products</i> , 2010, 73, 1434-1437. | 1.5 | 11 |
| 4932 | Synthesis and Structure of Intermediates in Copper-Catalyzed Alkylation of Diphenylphosphine. <i>Inorganic Chemistry</i> , 2010, 49, 7650-7662. | 1.9 | 56 |
| 4933 | Solvatochromic Shifts in Uracil: A Combined MD-QM/MM Study. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 249-256. | 2.3 | 66 |
| 4934 | Stilbene and Its Derivatives for Multistate Spectral Sensing. <i>IEEE Nanotechnology Magazine</i> , 2010, 9, 558-564. | 1.1 | 3 |
| 4935 | Theoretical Study of Formic Acid-Sulfur Dioxide Dimers. <i>Journal of Physical Chemistry A</i> , 2010, 114, 13182-13188. | 1.1 | 6 |
| 4936 | Transition Metal Intervention for a Classic Reaction: Assessing the Feasibility of Nickel(0)-Promoted [1,3] Sigmatropic Shifts of Bicyclo[3.2.0]hept-2-enes. <i>Organometallics</i> , 2010, 29, 3541-3545. | 1.1 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4937 | Formation of Acylsilenolates from Bis(acyl)trisilanes as the Silicon Analogues of Acylenolates. <i>Organometallics</i> , 2010, 29, 4199-4202. | 1.1 | 3 |
| 4938 | A QM/QM Multilayer Composite Methodology: The ONIOM Correlation Consistent Composite Approach (ONIOM-ccCA). <i>Journal of Physical Chemistry A</i> , 2010, 114, 9394-9397. | 1.1 | 17 |
| 4939 | Accounting for Polarization Cost When Using Fixed Charge Force Fields. I. Method for Computing Energy. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8621-8630. | 1.2 | 43 |
| 4940 | Comparative DFT Analysis of Ligand and Solvent Effects on the Mechanism of H ₂ Activation in Water Mediated by Half-Sandwich Complexes [Cp ² Ru(PTA) ₂ Cl] (Cp ² =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf <i>Organometallics</i> , 2010, 29, 5121-5131. | 1.1 | 32 |
| 4941 | Differentiating Mechanistic Possibilities for the Thermal, Intramolecular [2 + 2] Cycloaddition of Allene ² Ynes. <i>Journal of the American Chemical Society</i> , 2010, 132, 11952-11966. | 6.6 | 94 |
| 4942 | Understanding the Dynamics Behind the Photoisomerization of a Light-Driven Fluorene Molecular Rotary Motor. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5058-5067. | 1.1 | 96 |
| 4943 | Remarkable Reactions and Intermediates in Titanocene(IV) Chemistry: Migratory Insertion Reactions of 2,2-Disubstituted-1-alkenes, Intramolecular 1,5- σ Bond Metathesis via η^2 -Agostic Interactions, and a Rare Example of a η^2 -Agostic Alkyltitanocene Complex. <i>Journal of the American Chemical Society</i> , 2010, 132, 13357-13370. | 6.6 | 30 |
| 4944 | Formation of Aminyl Radicals on Electron Attachment to AZT: Abstraction from the Sugar Phosphate Backbone versus One-Electron Oxidation of Guanine. <i>Journal of Physical Chemistry B</i> , 2010, 114, 9289-9299. | 1.2 | 19 |
| 4945 | A DFT Study on the Mechanism of the Coupling Reaction between Chloromethyloxirane and Carbon Dioxide Catalyzed by Re(CO) ₅ Br. <i>Organometallics</i> , 2010, 29, 2069-2079. | 1.1 | 30 |
| 4946 | Caged Chalcogens: Theoretical Studies on a Tetracoordinated Oxonium Dication and Its Higher Homologues. <i>Organic Letters</i> , 2010, 12, 772-775. | 2.4 | 13 |
| 4947 | Direct Information on Structure and Energetic Features of Cu ⁺ Xe Species Formed in MFI-Type Zeolite at Room Temperature. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 2642-2650. | 2.1 | 20 |
| 4948 | Astatine Standard Redox Potentials and Speciation in Acidic Medium. <i>Journal of Physical Chemistry A</i> , 2010, 114, 576-582. | 1.1 | 65 |
| 4949 | Ligand Effects on the [Cu(PhO)(PhOH)] ⁺ Redox Active Complex. <i>Inorganic Chemistry</i> , 2010, 49, 8421-8429. | 1.9 | 18 |
| 4950 | Kinetics of hydrogen-transfer isomerizations of butoxyl radicals. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7782. | 1.3 | 151 |
| 4951 | Si ⁺ Ge-based Oxynitrides: From Molecules to Solids. <i>Chemistry of Materials</i> , 2010, 22, 3884-3899. | 3.2 | 9 |
| 4952 | Femtosecond to Microsecond Photochemistry of a [FeFe]hydrogenase Enzyme Model Compound. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15370-15379. | 1.2 | 34 |
| 4953 | Stille Cross-Coupling Reactions of Alkenylstannanes with Alkenyl Iodides Mediated by Copper(I) Thiophene-2-carboxylate: A Density Functional Study. <i>Organometallics</i> , 2010, 29, 3077-3084. | 1.1 | 34 |
| 4954 | Structure and Conformational Stability of Protonated Dialanine. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7537-7543. | 1.1 | 6 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 4955 | Hole Mobility for Thin-Film Organic Molecular Solids in the Presence of Defects or Surface Adsorbates: Theory and Implications for Gas Detection. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12173-12189. | 1.5 | 10 |
| 4956 | Scanning the Potential Energy Surface of Furanosyl Oxocarbenium Ions: Models for Reactive Intermediates in Glycosylation Reactions. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5180-5186. | 1.1 | 25 |
| 4957 | Holo-Ni(II)HpNikR Is an Asymmetric Tetramer Containing Two Different Nickel-Binding Sites. <i>Journal of the American Chemical Society</i> , 2010, 132, 14447-14456. | 6.6 | 36 |
| 4958 | Combined Effects of One 8-Hydroxyquinoline/Picolinate and α -CH β -N Substitutions on the Geometry, Electronic Structure and Optical Properties of <i>mer</i> -Alq ₃ . <i>Journal of Physical Chemistry A</i> , 2010, 114, 652-658. | 1.1 | 7 |
| 4959 | The Minnesota Density Functionals and their Applications to Problems in Mineralogy and Geochemistry. <i>Reviews in Mineralogy and Geochemistry</i> , 2010, 71, 19-37. | 2.2 | 35 |
| 4960 | Solid-State Density Functional Theory Investigation of the Terahertz Spectra of the Structural Isomers 1,2-Dicyanobenzene and 1,3-Dicyanobenzene. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12513-12521. | 1.1 | 44 |
| 4961 | Formation of Beyerene, Kaurene, Trachylobane, and Atiserene Diterpenes by Rearrangements That Avoid Secondary Carbocations. <i>Journal of the American Chemical Society</i> , 2010, 132, 5375-5386. | 6.6 | 77 |
| 4962 | Application of the Diffusion Monte Carlo Method to the Binding of Excess Electrons to Water Clusters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1364-1366. | 1.1 | 18 |
| 4963 | Binuclear terephthalato-bridged copper(II) complex with N ₂ O ₂ coordinating tripodal ligand: synthesis, structure, magnetic properties, and DFT study. <i>Journal of Coordination Chemistry</i> , 2010, 63, 1893-1903. | 0.8 | 5 |
| 4964 | Temperature Dependence of the 1,6-Diphenyl-1,3,5-hexatriene Triplet Lifetime in Solution and Theoretical Evaluation of Triplet Conformer Interconversion. <i>Journal of Physical Chemistry B</i> , 2010, 114, 14480-14486. | 1.2 | 3 |
| 4965 | The Role of Exact Exchange in the Description of Cu ²⁺ (H ₂ O) _n (n = 1-6) Complexes by Means of DFT Methods. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10857-10863. | 1.1 | 43 |
| 4966 | Improved Density Functional Description of the Electrochemistry and Structure-Property Descriptors of Substituted Flavins. <i>Journal of Physical Chemistry B</i> , 2010, 114, 14907-14915. | 1.2 | 34 |
| 4967 | Facile C-H Bond Cleavage via a Proton-Coupled Electron Transfer Involving a C-H...Cu ^{II} Interaction. <i>Journal of the American Chemical Society</i> , 2010, 132, 12299-12306. | 6.6 | 131 |
| 4968 | Interactions of Tetrahedrane and Tetrasilatetrahedrane with CH ₂ and SiH ₂ : A Computational Study. <i>Organometallics</i> , 2010, 29, 4975-4982. | 1.1 | 2 |
| 4969 | Acyclic Guanidines as Organic Catalysts for Living Polymerization of Lactide. <i>Macromolecules</i> , 2010, 43, 1660-1664. | 2.2 | 74 |
| 4970 | Gold(I)-Catalyzed Hydration of 1,2-Diphenylacetylene: Computational Insights. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2782-2789. | 2.3 | 16 |
| 4971 | Shielding Constants and Chemical Shifts in DFT: Influence of Optimized Effective Potential and Coulomb-Attenuation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7179-7186. | 1.1 | 18 |
| 4972 | Theoretical Study of the Mechanism of Valence Tautomerism in Cobalt Complexes. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12928-12935. | 1.1 | 49 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4973 | Theoretical Predictions of a New Family of Stable Bismuth and Other Group 15 Fullerenes. <i>Journal of Physical Chemistry C</i> , 2010, 114, 10775-10781. | 1.5 | 14 |
| 4974 | An Atomic-Orbital-Based Lagrangian Approach for Calculating Geometric Gradients of Linear Response Properties. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1028-1047. | 2.3 | 28 |
| 4975 | Stereoselective OsO ₄ -Catalyzed Oxidative Cyclization of 1,5-Dienes. <i>Journal of Organic Chemistry</i> , 2010, 75, 1967-1973. | 1.7 | 14 |
| 4976 | Diruthenium Phenylacetylide Complexes Bearing <i>para</i> -/ <i>meta</i> -Amino Phenyl Substituents. <i>Organometallics</i> , 2010, 29, 2783-2788. | 1.1 | 16 |
| 4977 | Theoretical Investigations on Reactions of a Series of Stable Dialkyl-Substituted Silicon-Chalcogen Doubly Bonded Compounds. <i>Organometallics</i> , 2010, 29, 527-535. | 1.1 | 5 |
| 4978 | Influence of Molecular Oxide Cages on Metal Carbonyls. <i>Journal of Physical Chemistry A</i> , 2010, 114, 987-993. | 1.1 | 2 |
| 4979 | Synthesis, Structures, and Dynamic Behavior of Intramolecularly Base-Stabilized Diphosphatetrylenes Containing a Five-Membered Chelate Ring. <i>Organometallics</i> , 2010, 29, 108-116. | 1.1 | 24 |
| 4980 | Mechanism for Hydride-Assisted Rearrangement from Ethylidene to Ethylene in Iridium Cationic Complexes. <i>Organometallics</i> , 2010, 29, 2040-2045. | 1.1 | 28 |
| 4981 | Microhydration of the Selenite Dianion: A Theoretical Study of Structures, Hydration Energies, and Electronic Stabilities of SeO ₃ ²⁻ (H ₂ O) _{<i>n</i>} (<i>n</i> = 6, 9) Clusters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8948-8960. | 1.1 | 8 |
| 4982 | Synthesis, Excited State Dynamics, and Optical Characteristics of Oligophenyl-Based Swivel Cruciforms in Solution and Solid State. <i>Journal of Physical Chemistry B</i> , 2010, 114, 12765-12776. | 1.2 | 5 |
| 4983 | The Quest for Tetracoordinated Halonium Ions: A Theoretical Investigation. <i>Organic Letters</i> , 2010, 12, 4844-4847. | 2.4 | 5 |
| 4984 | Photocatalytic Water Oxidation at the GaN (101̄...0)̄-Water Interface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13695-13704. | 1.5 | 74 |
| 4985 | High-Spin Manganese(II) Complexes of an Amido/Bis(Phosphine) PNP Ligand. <i>Inorganic Chemistry</i> , 2010, 49, 5328-5334. | 1.9 | 28 |
| 4986 | Transition-Metal-Doped Aluminum Hydrides as Building Blocks for Supramolecular Assemblies. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12318-12322. | 1.1 | 4 |
| 4987 | Structural and Dynamic Properties of the New Alternative Refrigerant 2,3,3,3-Tetrafluoro-1-propene (HFO-1234yf) in the Liquid State. <i>Journal of Physical Chemistry B</i> , 2010, 114, 17120-17127. | 1.2 | 11 |
| 4988 | A Paradigm for Blue- or Red-Shifted Absorption of Small Molecules Depending on the Site of π -Extension. <i>Journal of the American Chemical Society</i> , 2010, 132, 16247-16255. | 6.6 | 96 |
| 4989 | Theoretical Investigation on the Isomerization Reaction of 4-Phenyl-hexa-1,5-enyne Catalyzed by Homogeneous Au Catalysts. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12893-12899. | 1.1 | 33 |
| 4990 | Theoretical Investigation of the Oxidation of Propane by FeO ⁺ . <i>Journal of Physical Chemistry A</i> , 2010, 114, 2701-2709. | 1.1 | 9 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 4991 | Mechanism of the Cobalt Oxazoline Palladacycle (COP)-Catalyzed Asymmetric Synthesis of Allylic Esters. <i>Journal of the American Chemical Society</i> , 2010, 132, 15192-15203. | 6.6 | 58 |
| 4992 | Application of the SCC-DFTB Method to $H^{+}(H_2O)_6$, $H^{+}(H_2O)_{21}$, and $H^{+}(H_2O)_{22}$. <i>Journal of Physical Chemistry B</i> , 2010, 114, 6932-6936. | 1.2 | 30 |
| 4993 | Reaction Mechanism of the Gold(I)-Catalyzed Addition of Phenols to Olefins: A Concerted Process Accelerated by Phenol and Water. <i>Organometallics</i> , 2010, 29, 3252-3260. | 1.1 | 67 |
| 4994 | Complexation of Cm(III) with Fluoride in Aqueous Solution in the Temperature Range from 20 to 90 °C. A Joint TRLFS and Quantum Chemical Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15626-15634. | 1.2 | 15 |
| 4995 | Dinuclear Dicyclopentadienyl Titanium Complexes with Bridging Cyclopentadienylsiloxo Ligands. <i>Organometallics</i> , 2010, 29, 642-655. | 1.1 | 6 |
| 4996 | Synthesis of Gold Phosphido Complexes Derived from Bis(secondary) Phosphines. Structure of Tetrameric $[Au(MesP(CH_2)_3PMe)Au]_4$. <i>Inorganic Chemistry</i> , 2010, 49, 3950-3957. | 1.9 | 21 |
| 4997 | Structure and Excitonic Coupling in Self-Assembled Monolayers of Azobenzene-Functionalized Alkanethiols. <i>Journal of the American Chemical Society</i> , 2010, 132, 1831-1838. | 6.6 | 100 |
| 4998 | SEIRA and SERS Effects in Cyclopentabithiophenethiol-Capped Gold Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12900-12904. | 1.5 | 11 |
| 4999 | Molecular Driving Forces for Z/E Isomerization Mediated by Heteroatoms: The Example Hemithioindigo. <i>Journal of Physical Chemistry A</i> , 2010, 114, 13016-13030. | 1.1 | 58 |
| 5000 | Atomic Structure and Magnetic Nature of Copper Hydroxide Acetate. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20213-20219. | 1.5 | 7 |
| 5001 | Influence of Explicit Hydration Waters in Calculating the Hydrolysis Constants for Geochemically Relevant Metals. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1917-1925. | 1.1 | 40 |
| 5002 | An Assessment of Density Functional Methods for Potential Energy Curves of Nonbonded Interactions: The XYG3 and B97-D Approximations. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 727-734. | 2.3 | 91 |
| 5003 | Rational Design of Highly Cytotoxic η^6 -Arene η^2 -Diketiminato [−] Ruthenium Complexes. <i>Organometallics</i> , 2010, 29, 417-427. | 1.1 | 33 |
| 5004 | A System-Dependent Density-Based Dispersion Correction. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1990-2001. | 2.3 | 133 |
| 5005 | How an Enzyme Might Accelerate an Intramolecular Diels-Alder Reaction: Theozymes for the Formation of Salvileucalin B. <i>Organic Letters</i> , 2010, 12, 1164-1167. | 2.4 | 19 |
| 5006 | Importance of Equilibrium Fluctuations between Most Stable Conformers in the Control of the Reaction Mechanism. <i>Journal of Organic Chemistry</i> , 2010, 75, 7186-7193. | 1.7 | 14 |
| 5007 | Trends in R^X Bond Dissociation Energies ($R = Me, Et, i-Pr, t-Bu, X = H, Me, Cl, OH$). <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1462-1469. | 2.3 | 39 |
| 5008 | Electron Paramagnetic Resonance Studies of Nitrosyl and Thionitrosyl and Density Functional Theory Studies of Nitrido, Nitrosyl, Thionitrosyl, and Selenonitrosyl Complexes of Chromium. <i>Inorganic Chemistry</i> , 2010, 49, 8769-8778. | 1.9 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5009 | Synthesis and Characterization of Ruthenium(II) π -Pyridylamine Complexes with Catechol Pendants as Metal Binding Sites. <i>Inorganic Chemistry</i> , 2010, 49, 3737-3745. | 1.9 | 13 |
| 5010 | Computational Insights into the Mechanism of Porphobilinogen Synthase. <i>Journal of Physical Chemistry B</i> , 2010, 114, 16860-16870. | 1.2 | 17 |
| 5011 | Characterization of the Structures of Phosphodiesterase 10 Binding with Adenosine 3 α ,5 α -Monophosphate and Guanosine 3 α ,5 α -Monophosphate by Hybrid Quantum Mechanical/Molecular Mechanical Calculations. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7022-7028. | 1.2 | 8 |
| 5012 | Theoretical Investigation of the Mechanism and Dynamics of Intramolecular Coherent Resonance Energy Transfer in Soft Molecules: A Case Study of Dithia-anthracenophane. <i>Journal of the American Chemical Society</i> , 2010, 132, 16911-16921. | 6.6 | 24 |
| 5013 | Theoretical and Raman Spectroscopic Studies of Phenolic Lignin Model Monomers. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8009-8021. | 1.2 | 86 |
| 5014 | Site-specific Xe additions into Cu α -ZSM-5 zeolite. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2392. | 1.3 | 32 |
| 5015 | Synthesis and X-ray Structure of a Diamagnetic Oxo-Bridged Trifluoromethyl π -Chromium(V) Complex: Structural and Computational Comparisons between CF ₃ and CH ₃ Ligands in Two Different Oxidation States of Chromium. <i>Organometallics</i> , 2010, 29, 3672-3675. | 1.1 | 10 |
| 5016 | Computation of Nonretarded London Dispersion Coefficients and Hamaker Constants of Copper Phthalocyanine. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 491-498. | 2.3 | 8 |
| 5017 | Multi-Length Scale Morphology of Poly(ethylene oxide)-Based Sulfonate Ionomers with Alkali Cations at Room Temperature. <i>Macromolecules</i> , 2010, 43, 4223-4229. | 2.2 | 76 |
| 5018 | Aggregation Behavior of a Conjugated C ₃ -Symmetric Molecule: A Description Based on Chiro-Optical Experimental and Theoretical Spectroscopies. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5710-5717. | 1.2 | 7 |
| 5019 | Reaction Mechanisms for Graphene and Carbon Nanotube Fluorination. <i>Journal of Physical Chemistry C</i> , 2010, 114, 3340-3345. | 1.5 | 56 |
| 5020 | Cascade [1,3]-Sigmatropic Rearrangements of Ketene $\langle i \rangle O \langle /i \rangle$, $\langle i \rangle O \langle /i \rangle$ -Acetals: Kinetic and DFT Level Mechanistic Studies. <i>Journal of Organic Chemistry</i> , 2010, 75, 1898-1910. | 1.7 | 6 |
| 5021 | Optimizing the Synthesis of Nitrogen-Substituted Zeolites. <i>Chemistry of Materials</i> , 2010, 22, 130-142. | 3.2 | 22 |
| 5022 | Influence of Hydrogen Bonds on the Stability of Some Cationic Monoaminocarbene Tantalum Complexes Containing Tridentate Bis(phenolato) [OSO]-Type Ligands. <i>Organometallics</i> , 2010, 29, 5834-5840. | 1.1 | 9 |
| 5023 | H-Bonding-Assisted Substituent Effect. <i>Journal of Organic Chemistry</i> , 2010, 75, 4944-4949. | 1.7 | 45 |
| 5024 | Unprecedented Near-Infrared (NIR) Emission in Diplatinum(III) (d ⁷ d ⁷) Complexes at Room Temperature. <i>Journal of the American Chemical Society</i> , 2010, 132, 7094-7103. | 6.6 | 53 |
| 5025 | Thermochemical benchmarking of hydrocarbon bond separation reaction energies: Jacob's ladder is not reversed!. <i>Molecular Physics</i> , 2010, 108, 2655-2666. | 0.8 | 53 |
| 5026 | The R.E.D. tools: advances in RESP and ESP charge derivation and force field library building. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7821. | 1.3 | 778 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5027 | Locked chromophores as CD and NMR probes for the helical conformation of tetraamidic macrocycles. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 1807. | 1.5 | 27 |
| 5028 | A Five-Coordinate [2Fe ^{II} 2S] Cluster. <i>Inorganic Chemistry</i> , 2010, 49, 5853-5858. | 1.9 | 16 |
| 5029 | Theoretical study of H ₂ splitting and storage by boron–nitrogen-based systems: a bimolecular case and some qualitative aspects. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 149-155. | 1.3 | 18 |
| 5030 | How Well Can Kohn–Sham DFT Describe the HO ₂ + O ₃ Reaction?. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2751-2761. | 2.3 | 21 |
| 5031 | The biphenyl-monitored effective size of unsaturated functional or fluorinated ortho substituents. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 4463. | 1.5 | 38 |
| 5032 | Nuclear-Electronic Orbital Method within the Fragment Molecular Orbital Approach. <i>Journal of Physical Chemistry C</i> , 2010, 114, 5582-5588. | 1.5 | 16 |
| 5033 | Synthesis and Electronic Structure of Tetrakis(<i>i</i> -propylphenylpropargyl)zirconium. <i>Organometallics</i> , 2010, 29, 5252-5256. | 1.1 | 9 |
| 5034 | Density functional theory study and kinetic analysis of the formation mechanism of Al ₃ O ₈ (OH) ₅ (H ₂ O) ₂₆ 18+ (Al ₃ O) in aqueous solution. <i>Geochimica Et Cosmochimica Acta</i> , 2010, 74, 1220-1229. | 1.6 | 18 |
| 5035 | The role of structural chemistry in the inhibitive performance of some aminopyrimidines on the corrosion of steel. <i>Corrosion Science</i> , 2010, 52, 2387-2396. | 3.0 | 165 |
| 5036 | Dipole assisted exciton dissociation at conjugated polymer/fullerene photovoltaic interfaces: A molecular study using density functional theory calculations. <i>Synthetic Metals</i> , 2010, 160, 643-650. | 2.1 | 98 |
| 5037 | E-Type Delayed Fluorescence of a Phosphine-Supported Cu ₂ (1,4-NAr ₂) ₂ Diamond Core: Harvesting Singlet and Triplet Excitons in OLEDs. <i>Journal of the American Chemical Society</i> , 2010, 132, 9499-9508. | 6.6 | 445 |
| 5038 | Determination of the absolute configurations of bicyclo[3.1.0]hexane derivatives via electronic circular dichroism, optical rotation dispersion and vibrational circular dichroism spectroscopy and density functional theory calculations. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 3777. | 1.5 | 20 |
| 5039 | On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2071-2085. | 2.3 | 383 |
| 5040 | Density functional approximations for charge transfer excitations with intermediate spatial overlap. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 12697. | 1.3 | 101 |
| 5041 | Internal Proton Transfer in the External Pyridoxal 5'-Phosphate Schiff Base in Dopa Decarboxylase. <i>Biochemistry</i> , 2010, 49, 84-94. | 1.2 | 37 |
| 5042 | EPR and ENDOR Studies of Dimeric Paracyclophane Radical Cations and Dications Containing Tri- and Pentamethylene-Bridged p-Phenylene Diamine Units. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6487-6492. | 1.1 | 14 |
| 5043 | [2 + 2] Photocycloaddition of 2(<i>H</i>)-Furanone to Unsaturated Compounds. Insights from First Principles Calculations and Transient-Absorption Measurements. <i>Journal of Organic Chemistry</i> , 2010, 75, 4392-4401. | 1.7 | 17 |
| 5044 | Structural metastability of endohedral silicon fullerenes. <i>Physical Review B</i> , 2010, 81, . | 1.1 | 39 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 5045 | Accounting for Polarization Cost When Using Fixed Charge Force Fields. II. Method and Application for Computing Effect of Polarization Cost on Free Energy of Hydration. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8631-8645. | 1.2 | 32 |
| 5046 | Interaction of Ketocyanine Dye with a Co^{2+} Ion: An Electronic Spectroscopic Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10388-10394. | 1.1 | 7 |
| 5047 | Chiral oxorhenium(v) complexes as candidates for the experimental observation of molecular parity violation: a structural, synthetic and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8792. | 1.3 | 20 |
| 5048 | Formulations of the closed-shell interactions in endohedral systems. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6187. | 1.3 | 29 |
| 5049 | The carbocation continuum in terpene biosynthesis—where are the secondary cations?. <i>Chemical Society Reviews</i> , 2010, 39, 2847. | 18.7 | 147 |
| 5050 | Experimental and Computational Thermochemical Study of Sulfur-Containing Amino Acids: L -Cysteine, L -Cystine, and L -Cysteine-Derived Radicals. $\text{S}^{\bullet}\text{S}$, $\text{S}^{\bullet}\text{H}$, and $\text{C}^{\bullet}\text{S}$ Bond Dissociation Enthalpies. <i>Journal of Physical Chemistry B</i> , 2010, 114, 10530-10540. | 1.2 | 46 |
| 5051 | A benchmark study of the vertical electronic spectra of the linear chain radicals C_2H and C_4H . <i>Journal of Chemical Physics</i> , 2010, 132, 144303. | 1.2 | 40 |
| 5052 | Cr^{III} Interactions in Two Alkoxo-Bridged Heterometallic Zn_2Cr_2 Complexes Self-Assembled from Zinc Oxide, Reinecke's Salt, and Diethanolamine. <i>Inorganic Chemistry</i> , 2010, 49, 5460-5471. | 1.9 | 42 |
| 5053 | Perchloric Acid Catalyzed Homogeneous and Heterogeneous Addition of I_2 -Dicarbonyl Compounds to Alcohols and Alkenes and Investigation of the Mechanism. <i>Journal of Organic Chemistry</i> , 2010, 75, 5017-5030. | 1.7 | 30 |
| 5054 | Describing Anions by Density Functional Theory: Fractional Electron Affinity. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2726-2735. | 2.3 | 104 |
| 5055 | Radical formation of amino acid precursors in interstellar regions? Ser, Cys and Asp. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 4934. | 1.5 | 11 |
| 5056 | Molecular Engineering of Benzothiazolium Salts with Large Quadratic Hyperpolarizabilities: Can Auxiliary Electron-Withdrawing Groups Enhance Nonlinear Optical Responses?. <i>Journal of Physical Chemistry C</i> , 2010, 114, 22289-22302. | 1.5 | 111 |
| 5057 | Theoretical Study on Conformation and Electronic State of $\text{H}^{\text{A}1/4}\text{ckel}$ -Aromatic Multiply N-Confused [26]Hexaphyrins. <i>Journal of Organic Chemistry</i> , 2010, 75, 8213-8223. | 1.7 | 32 |
| 5058 | Dissecting a Dyotropic Rearrangement. <i>Journal of Organic Chemistry</i> , 2010, 75, 1693-1700. | 1.7 | 23 |
| 5059 | Assessing the Performance of Popular Quantum Mechanics and Molecular Mechanics Methods and Revealing the Sequence-Dependent Energetic Features Using 100 Tetrapeptide Models. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1199-1209. | 2.3 | 42 |
| 5060 | Atomistic modeling of interfaces and their impact on microstructure and properties. <i>Acta Materialia</i> , 2010, 58, 1117-1151. | 3.8 | 430 |
| 5061 | Effect of the Substituent and Hydrogen Bond on the Geometry and Electronic Properties of OH and O^{\bullet} Groups in <i>para</i> -Substituted Phenol and Phenolate Derivatives. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10885-10890. | 1.1 | 14 |
| 5062 | Electronic Structure of an Iron-Porphyrin Nitrene Complex. <i>Inorganic Chemistry</i> , 2010, 49, 243-248. | 1.9 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5063 | Hybrid functional study of proper and improper multiferroics. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5405. | 1.3 | 147 |
| 5064 | Self-Assembly of Structurally Persistent Micelles Is Controlled by Specific-Ion Effects and Hydrophobic Guests. <i>Langmuir</i> , 2010, 26, 10460-10466. | 1.6 | 22 |
| 5065 | Ligand Exchange Processes on the Solvated Zinc Cation II. $[Zn(H_2O)_4L]^{2+} \cdot 2H_2O$ with $L = NH_3, NH_2(CH_3), NH(CH_3)_2,$ and $N(CH_3)_3$. <i>Australian Journal of Chemistry</i> , 2010, 63, 236. | 0.5 | 13 |
| 5066 | Structure and Energetics of C60O: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1939-1943. | 1.1 | 15 |
| 5067 | Single-particle and quasiparticle interpretation of Kohn-Sham and generalized Kohn-Sham eigenvalues for hybrid functionals. <i>Physical Review B</i> , 2010, 82, . | 1.1 | 58 |
| 5068 | Substituent Effects on the Electron Affinities and Ionization Energies of Tri-, Penta-, and Heptafulvenes: A Computational Investigation. <i>Journal of Organic Chemistry</i> , 2010, 75, 8060-8068. | 1.7 | 30 |
| 5069 | Clar's Theory, π -Electron Distribution, and Geometry of Graphene Nanoribbons. <i>Journal of the American Chemical Society</i> , 2010, 132, 3440-3451. | 6.6 | 219 |
| 5070 | Ridge-Tile-like Chiral Topology: Synthesis, Resolution, and Complete Chiroptical Characterization of Enantiomers of Edge-Sharing Binuclear Square Planar Complexes of Ni(II) Bearing Achiral Ligands. <i>Journal of the American Chemical Society</i> , 2010, 132, 10477-10483. | 6.6 | 41 |
| 5071 | Nature of Bonding in Group 13 Dimetalenes: a Delicate Balance between Singlet Diradical Character and Closed Shell Interactions. <i>Inorganic Chemistry</i> , 2010, 49, 10992-11000. | 1.9 | 45 |
| 5072 | An Improved Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) Set of Parameters for Simulation of Bulk and Molecular Systems Involving Titanium. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 266-278. | 2.3 | 177 |
| 5073 | QM/MM Studies of Xanthine Oxidase: Variations of Cofactor, Substrate, and Active-Site Glu802. <i>Journal of Physical Chemistry B</i> , 2010, 114, 1506-1517. | 1.2 | 29 |
| 5074 | Relativistic Density Functional Theory. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2010, , 191-214. | 0.6 | 13 |
| 5075 | Experimental and theoretical study on activation of the C-H bond in pyridine by $[Mm]^{+}$ ($M = Cu, Ag, Au$). <i>TJ ETQ 0 0 0 rg BT /Overloc</i> | 1.3 | 5 |
| 5076 | Adsorption Behaviors of 4-Mercaptobenzoic Acid on Silver and Gold Films. <i>Chinese Journal of Chemical Physics</i> , 2010, 23, 659-663. | 0.6 | 30 |
| 5077 | Stereoselectivity in oxallyl-furan (4 + 3) cycloadditions: control of intermediate conformations and dispersive stabilisation in cycloadditions involving oxazolidinone auxiliaries. <i>Chemical Science</i> , 2010, 1, 387. | 3.7 | 62 |
| 5078 | Insights into the structure and stability of the carbonic acid dimer. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10963. | 1.3 | 50 |
| 5079 | Reactive Molecular Dynamics Studies of DMMP Adsorption and Reactivity on Amorphous Silica Surfaces. <i>Journal of Physical Chemistry C</i> , 2010, 114, 18894-18902. | 1.5 | 61 |
| 5080 | Efficient Diffuse Basis Sets for Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 597-601. | 2.3 | 138 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5081 | Copper-Catalyzed Enantioselective Propargylic Amination of Propargylic Esters with Amines: Copper π -Allenylidene Complexes as Key Intermediates. <i>Journal of the American Chemical Society</i> , 2010, 132, 10592-10608. | 6.6 | 198 |
| 5082 | Frontiers in electronic structure theory. <i>Journal of Chemical Physics</i> , 2010, 132, 110902. | 1.2 | 147 |
| 5083 | Modeling the Charge Transfer between Alkali Metals and Polycyclic Aromatic Hydrocarbons Using Electronic Structure Methods. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10326-10333. | 1.1 | 53 |
| 5084 | Computational Studies of the Isomerization and Hydration Reactions of Acetaldehyde Oxide and Methyl Vinyl Carbonyl Oxide. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9192-9204. | 1.1 | 117 |
| 5085 | Stereomutation of Axially Chiral Aryl Coumarins. <i>Journal of Organic Chemistry</i> , 2010, 75, 5927-5933. | 1.7 | 30 |
| 5086 | Origins of Stereoselectivity in the α -Alkylation of Chiral Hydrazones. <i>Journal of Organic Chemistry</i> , 2010, 75, 8578-8584. | 1.7 | 30 |
| 5087 | Electronic structure and properties of isoelectronic magic clusters: Al_3X^{\pm} (X=H,Au,Li,Na,K,Rb,Cs). <i>Journal of Chemical Physics</i> , 2010, 133, 124308. | 1.2 | 40 |
| 5088 | A charge-transfer surface enhanced Raman scattering model from time-dependent density functional theory calculations on a Ag ₁₀ -pyridine complex. <i>Journal of Chemical Physics</i> , 2010, 132, 214707. | 1.2 | 64 |
| 5089 | Mechanism of the Swern Oxidation: Significant Deviations from Transition State Theory. <i>Journal of Organic Chemistry</i> , 2010, 75, 8088-8099. | 1.7 | 23 |
| 5090 | Charge Transport in Organic Crystals: Role of Disorder and Topological Connectivity. <i>Journal of the American Chemical Society</i> , 2010, 132, 11702-11708. | 6.6 | 157 |
| 5091 | Ferrocene-like iron bis(dicarbollide), $[3-Fe^{III}(1,2-C_2B_9H_{11})_2]^{+}$. The first experimental and theoretical refinement of a paramagnetic ¹¹ B NMR spectrum. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7018. | 1.3 | 25 |
| 5092 | The solid state structure and reactivity of NbCl ₅ ·(N,N ϵ ² -dicyclohexylurea) in solution: evidence for co-ordinated urea dehydration to the relevant carbodiimide. <i>Dalton Transactions</i> , 2010, 39, 6985. | 1.6 | 31 |
| 5093 | Theoretical Elucidation of Au(I)-Catalyzed Cycloisomerizations of Cycloalkyl-substituted 1,5-Enynes: 1,2-alkyl Shift versus C α -H Bond Insertion Products. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6164-6170. | 1.1 | 42 |
| 5094 | Stable and Tunable Phosphorescent Neutral Cyclometalated Au(III) Diaryl Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 11463-11472. | 1.9 | 78 |
| 5095 | Mechanistic Insights into Alkene Epoxidation with H ₂ O ₂ by Ti- and other TM-Containing Polyoxometalates: Role of the Metal Nature and Coordination Environment. <i>Journal of the American Chemical Society</i> , 2010, 132, 7488-7497. | 6.6 | 148 |
| 5096 | Improved Description of the Structure of Molecular and Layered Crystals: Ab Initio DFT Calculations with van der Waals Corrections. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11814-11824. | 1.1 | 895 |
| 5097 | The Linear Response Kernel: Inductive and Resonance Effects Quantified. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 1228-1234. | 2.1 | 74 |
| 5098 | Ab Initio Study of Xe Adsorption on Graphene. <i>Journal of Physical Chemistry C</i> , 2010, 114, 3544-3548. | 1.5 | 55 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5099 | [2 + 2] Cycloaddition of Carbon Disulfide to NCN-Chelated δ -Organoantimony(III) and Organobismuth(III) Sulfides: Evidence for Terminal Sb δ -S and Bi δ -S Bonds in Solution δ . <i>Organometallics</i> , 2010, 29, 4486-4490. | 1.1 | 40 |
| 5100 | The binding of vitamin B12 to transcobalamin(II); structural considerations for bioconjugate design δ a molecular dynamics study. <i>Molecular BioSystems</i> , 2010, 6, 1611. | 2.9 | 15 |
| 5101 | Short-time Fourier transform analysis of real-time time-dependent Hartree δ -Fock and time-dependent density functional theory calculations with Gaussian basis functions. <i>Journal of Chemical Physics</i> , 2010, 132, 054104. | 1.2 | 34 |
| 5102 | Synthesis and characterisation of the persistent radical [BCl2(bipy)] δ ™. <i>Chemical Communications</i> , 2010, 46, 5070. | 2.2 | 29 |
| 5103 | Ethanolysis of N-substituted norbornane epoxyimides: Discovery of diverse pathways depending on substituent's character. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 2142-57. | 1.5 | 9 |
| 5104 | Solvent Effects on the Physicochemical Properties of the Cross-Linked Histidine δ -Tyrosine Ligand of Cytochrome c Oxidase. <i>Journal of Physical Chemistry B</i> , 2010, 114, 6409-6425. | 1.2 | 4 |
| 5105 | Synthesis and structural characterisation of germanium(ii) halide complexes with neutral N-donor ligands. <i>Dalton Transactions</i> , 2010, 39, 847-856. | 1.6 | 55 |
| 5106 | Unusual azobenzene/bipyridine palladacycles: structural, dynamical, photophysical and theoretical studies. <i>Dalton Transactions</i> , 2010, 39, 8769. | 1.6 | 26 |
| 5107 | Orbital-dependent Representation of Correlation Energy Functional. <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 455-466. | 1.4 | 2 |
| 5108 | Charge Transfer Interaction and Terahertz Studies of a Nonlinear Optical Material δ -Glutamine Picrate: A DFT Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 13055-13064. | 1.1 | 26 |
| 5109 | How Does Energized NCCCCCN Lose Carbon in the Gas Phase? A Joint Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 949-955. | 1.1 | 1 |
| 5110 | Computational Study of Alkynes Insertion into Metal-Hydride Bonds Catalyzed by Bimetallic Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 9875-9883. | 1.9 | 18 |
| 5111 | Hyperfine coupling constants of the nitrogen and phosphorus atoms: A challenge for exact-exchange density-functional and post-Hartree δ -Fock methods. <i>Journal of Chemical Physics</i> , 2010, 132, 184107. | 1.2 | 15 |
| 5112 | RECENT DEVELOPMENTS IN BIAXIAL LIQUID CRYSTALS: AN NMR PERSPECTIVE. <i>International Journal of Modern Physics B</i> , 2010, 24, 4641-4682. | 1.0 | 24 |
| 5113 | Synthesis, Structures, Photoluminescent Behaviors, and DFT Studies of Novel Aluminum Complexes Containing Phenoxybenzotriazole Derivatives. <i>Organometallics</i> , 2010, 29, 347-353. | 1.1 | 16 |
| 5114 | Validation of Density Functional Methods for the Calculation of Small Gold Clusters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10297-10308. | 1.1 | 43 |
| 5115 | Density Functional Calculations of E2 and S δ N δ 2 Reactions: Effects of the Choice of Density Functional, Basis Set, and Self-Consistent Iterations. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1104-1108. | 2.3 | 45 |
| 5116 | Role of dispersive interactions in the CO adsorption on MgO(001): periodic B3LYP calculations augmented with an empirical dispersion term. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6382. | 1.3 | 60 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5117 | Benzothiazole-Based Fluorophores of Donor–Acceptor–Donor Type Displaying High Two-Photon Absorption. <i>Journal of Organic Chemistry</i> , 2010, 75, 3053-3068. | 1.7 | 135 |
| 5118 | Synthesis and Photophysical Properties of N-Fused Tetraphenylporphyrin Derivatives: Near-Infrared Organic Dye of [18]Annulenic Compounds. <i>Journal of Organic Chemistry</i> , 2010, 75, 8637-8649. | 1.7 | 46 |
| 5119 | Partitioning of the molecular density matrix over atoms and bonds. <i>Journal of Chemical Physics</i> , 2010, 132, 164111. | 1.2 | 21 |
| 5120 | B3LYP calculations of cerium oxides. <i>Journal of Chemical Physics</i> , 2010, 132, 054110. | 1.2 | 65 |
| 5121 | Quantum chemical study of benzimidazole derivatives to tune the second-order nonlinear optical molecular switching by proton abstraction. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4791. | 1.3 | 106 |
| 5122 | Uracil anion radical in aqueous solution: thermodynamics versus spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10736. | 1.3 | 9 |
| 5123 | Photophysical and structural properties of the fluorescent nucleobase analogues of the tricyclic cytosine (tC) family. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8881. | 1.3 | 40 |
| 5124 | Hydrogen bonding to carbonyl hydride complex Cp*Mo(PMe ₃) ₂ (CO)H and its role in proton transfer. <i>Dalton Transactions</i> , 2010, 39, 2008. | 1.6 | 18 |
| 5125 | A tangled web of interconnecting pathways to amorphadiene and the amorphene sesquiterpenes. <i>Chemical Science</i> , 2010, 1, 609. | 3.7 | 32 |
| 5126 | Dialkylamino cyclopentadienyl ruthenium complex-catalyzed α -alkylation of arylacetonitriles with primary alcohols. <i>Dalton Transactions</i> , 2010, 39, 265-274. | 1.6 | 30 |
| 5127 | Prototropic equilibria in DNA containing one-electron oxidized GC: intra-duplex vs. duplex to solvent deprotonation. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5353. | 1.3 | 54 |
| 5128 | Molecular mechanism of acid-triggered aryl halide reductive elimination in well-defined aryl Cu(I) halide species. <i>Dalton Transactions</i> , 2010, 39, 10458. | 1.6 | 41 |
| 5129 | Adsorption-induced structural changes of gold cations from two- to three-dimensions. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 3038. | 1.3 | 20 |
| 5130 | Reactivity of the α -AlF ₃ (100) surface: defects, fluorine mobility and catalysis of the CCl ₂ F ₂ dismutation reaction. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6124. | 1.3 | 10 |
| 5131 | Synthesis, structure, and electronic properties of 4H-germanium. <i>Journal of Materials Chemistry</i> , 2010, 20, 1780. | 6.7 | 33 |
| 5132 | Existence of dual species composed of Cu ⁺ in CuMFI being bridged by C ₂ H ₂ . <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6455. | 1.3 | 25 |
| 5133 | Infra-red and Raman spectroscopy of free-base and zinc phthalocyanines isolated in matrices. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10406. | 1.3 | 49 |
| 5134 | Identification of the mechanism of enhanced exciton interaction in rigidly linked naphthalene dimers. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13070. | 1.3 | 10 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5135 | Matrix isolation studies on the co-condensation reactions of molecular SiO and GeO: the characterisation of the novel cyclic species SiGeO ₂ , Si ₂ GeO ₃ and SiGe ₂ O ₃ . <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6157. | 1.3 | 1 |
| 5136 | Towards understanding a mechanism for reversible hydrogen storage: theoretical study of transition metal catalysed dehydrogenation of sodium alanate. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4012. | 1.3 | 20 |
| 5137 | Synthesis, characterization and reactivity of carbohydrate platinum(iv) complexes with thioglycoside ligands. <i>Dalton Transactions</i> , 2010, 39, 6327. | 1.6 | 15 |
| 5138 | Silyloxyazadienes: one intermediate and two competitive pericyclic reactions. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5067. | 1.3 | 4 |
| 5139 | Structural, MALDI-TOF-MS, Magnetic and Spectroscopic Studies of New Dinuclear Copper(ii), Cobalt(ii) and Zinc(ii) Complexes Containing a Biomimicking μ_4 -OH bridge. <i>Dalton Transactions</i> , 2010, 39, 11654. | 1.6 | 16 |
| 5140 | Thioxanthone: on the shape of the first absorption band. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9320. | 1.3 | 14 |
| 5141 | Enantiomers of conformation-flexible cyclopentane-1,2,3,4-tetracarboxylate in metal-organic frameworks. <i>CrystEngComm</i> , 2010, 12, 4416. | 1.3 | 10 |
| 5142 | Effects of the silicon core structures on the hole mobility of star-shaped oligothiophenes. <i>Dalton Transactions</i> , 2010, 39, 9314. | 1.6 | 12 |
| 5143 | Carotenoids can act as antioxidants by oxidizing the superoxideradical anion. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 193-200. | 1.3 | 105 |
| 5144 | Femtosecond spectroscopy on the photochemistry of ortho-nitrotoluene. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 15653. | 1.3 | 43 |
| 5145 | Folding oligomers of difluorinated thienylfurans: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 523-532. | 1.3 | 5 |
| 5146 | On the calculation of the vibrational frequencies of polycyclic aromatic hydrocarbons. <i>Molecular Physics</i> , 2010, 108, 2647-2654. | 0.8 | 29 |
| 5147 | Combining the chemistries of silylene and sulfur-nitrogen compounds SiS_2N_2 and related systems. <i>Dalton Transactions</i> , 2010, 39, 3256. | 1.6 | 4 |
| 5148 | Improvement of cytotoxicity of titanocene-functionalized mesoporous materials by the increase of the titanium content. <i>Dalton Transactions</i> , 2010, 39, 2597. | 1.6 | 47 |
| 5149 | Formation of nitriles and imines in the atmosphere of Titan: combined crossed-beam and theoretical studies on the reaction dynamics of excited nitrogen atoms N(2D) with ethane. <i>Faraday Discussions</i> , 2010, 147, 189. | 1.6 | 79 |
| 5150 | Constrained Excited-State Structure in Molecular Crystals by Means of the QM/MM Approach: Toward the Prediction of Photocrystallographic Results. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 2349-2353. | 2.1 | 25 |
| 5151 | Ion Chemistry of VX Surrogates and Ion Energetics Properties of VX: New Suggestions for VX Chemical Ionization Mass Spectrometry Detection. <i>Analytical Chemistry</i> , 2010, 82, 3764-3771. | 3.2 | 13 |
| 5152 | Definitive Band Gaps for Single-Wall Carbon Nanotubes. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 2946-2950. | 2.1 | 179 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5153 | Tetratungsten Oxide Clusters W_4O_{n+10} ($n = 10\sim 13$): Structural Evolution and Chemical Bonding. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1964-1972. | 1.1 | 23 |
| 5154 | Calculation of One- and Two-Photon Absorption Spectra of Thiolated Gold Nanoclusters using Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2809-2821. | 2.3 | 47 |
| 5155 | Regioselectivities of (4 + 3) Cycloadditions between Furans and Oxazolidinone-Substituted Oxyallyls. <i>Organic Letters</i> , 2010, 12, 5506-5509. | 2.4 | 34 |
| 5156 | 1,4-Dihydro-1,4-diarsinine-Bridged Dinuclear <i>trans</i> -Dihaloplatinum(II) Complexes: Synthesis and Controlled Pt \sim Pt Interaction by Halogen Substitution Induced Conformational Change. <i>Organometallics</i> , 2010, 29, 4992-5003. | 1.1 | 12 |
| 5157 | Hydroquinoid Chromium Complexes Bearing an Acyclic Conjugated Bridge: Chromium-Templated Synthesis, Molecular Structure, and Haptotropic Metal Migration. <i>Organometallics</i> , 2010, 29, 6172-6185. | 1.1 | 11 |
| 5158 | Mechanistic Investigation of the Hydrogenation of O_2 by a Transfer Hydrogenation Catalyst. <i>Journal of the American Chemical Society</i> , 2010, 132, 4178-4190. | 6.6 | 34 |
| 5159 | Quantum Chemical Study on Ethylene Addition to $(O\sim)_2Os(\sim NH)_2$ and $(O\sim)_2Os(\sim NH)-cyclo-(\sim NHCH_2)_2CH_2HN\sim$ as Model Complexes for the Osmium-Catalyzed Aminohydroxylation of Olefins. <i>Organometallics</i> , 2010, 29, 1560-1568. | 1.1 | 7 |
| 5160 | Tuning the electronic properties of dppz-ligands and their palladium(ii) complexes. <i>Dalton Transactions</i> , 2010, 39, 4331. | 1.6 | 33 |
| 5161 | Assessment of the performance of common density functional methods for describing the interaction energies of $(H_2O)_6$ clusters. <i>Journal of Chemical Physics</i> , 2010, 132, 134303. | 1.2 | 66 |
| 5162 | First-principles study of oxygen vacancies in MgO . <i>Physical Review B</i> , 2010, 81, 114107. | 1.1 | 13 |
| 5163 | On the nature of homo- and hetero-dinuclear metal \sim metal quadruple bonds \sim Analysis of the bonding situation and benchmarking DFT against wave function methods. <i>Canadian Journal of Chemistry</i> , 2010, 88, 1079-1093. | 0.6 | 22 |
| 5164 | Microsolvation of the formic acid dimer \sim $(HCOOH)_2(H_2O)_n$ clusters with $n = 1, \dots, 5$. <i>Canadian Journal of Chemistry</i> , 2010, 88, 736-743. | 0.6 | 8 |
| 5165 | Vibrational Spectroscopic and Theoretical Studies of Urea Derivatives with Biochemical Interest: <i>N,N</i> -Dimethylurea, <i>N,N</i> -Tetramethylurea, and <i>N,N</i> -Dimethylpropyleneurea. <i>Applied Spectroscopy Reviews</i> , 2010, 45, 274-326. | 3.4 | 10 |
| 5166 | Mass-spectrometric and computational study of tryptophan radicals $(Trp + H)^{\dot{E}}$ produced by collisional electron transfer to protonated tryptophan in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13434. | 1.3 | 17 |
| 5167 | Exploring wavepacket dynamics behind strong-field momentum-dependent photodissociation in CH_2BrI^+ . <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 14203. | 1.3 | 37 |
| 5168 | Terminal versus bridging cyclobutadiene rings in binuclear nickel carbonyl derivatives: A cube-antiprism twist of the cyclobutadiene rings in the perpendicular structures. <i>New Journal of Chemistry</i> , 2010, 34, 1885. | 1.4 | 4 |
| 5169 | Counterion-dependent deuteration of pentamethylcyclopentadiene in water-soluble cationic Rh(III) complexes assisted by PTA. <i>Dalton Transactions</i> , 2010, 39, 3366. | 1.6 | 20 |
| 5170 | A vibrational circular dichroism approach to the determination of the absolute configuration of flexible and transparent molecules: fluorenone ketals of 1,n-diols. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4725. | 1.3 | 12 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5171 | Melem- and melamine-derived iminophosphanes. <i>New Journal of Chemistry</i> , 2010, 34, 1893. | 1.4 | 25 |
| 5172 | Bipolar redox behaviour, field-effect mobility and transistor switching of the low-molecular azo glass AZOPD. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13828. | 1.3 | 15 |
| 5173 | Fluorescence sensing of caffeine in water with polysulfonated pyrenes. <i>Chemical Communications</i> , 2011, 47, 10584. | 2.2 | 43 |
| 5174 | Theoretical studies on the mechanism and stereoselectivity of Rh(Phebox)-catalyzed asymmetric reductive aldol reaction. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 5845. | 1.5 | 26 |
| 5175 | Relativistic effects on group-12 metal nuclear shieldings. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 21016. | 1.3 | 35 |
| 5176 | Doubly hybrid density functional for accurate description of thermochemistry, thermochemical kinetics and nonbonded interactions. <i>International Reviews in Physical Chemistry</i> , 2011, 30, 115-160. | 0.9 | 116 |
| 5177 | On the dimerization of chlorophyll in photosystem II. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16022. | 1.3 | 17 |
| 5178 | Adequate representation of charge polarization effects leads to a successful treatment of the CF ₄ + SiCl ₄ + CCl ₄ + SiF ₄ reaction by density functional theory. <i>Chemical Communications</i> , 2011, 47, 2357-2359. | 2.2 | 4 |
| 5179 | Exchange coupling through diamagnetic [Fe(CO) ₄] ₂ bridging ligands in a xenophilic cluster. <i>Dalton Transactions</i> , 2011, 40, 927-932. | 1.6 | 3 |
| 5180 | Switching of excited states in cyclometalated platinum complexes incorporating pyridyl-acetylide ligands (Pt-C≡C-py): a combined experimental and theoretical study. <i>New Journal of Chemistry</i> , 2011, 35, 2196. | 1.4 | 25 |
| 5181 | Mechanistic Insight into Protonolysis and Cis-Trans Isomerization of Benzylplatinum(II) Complexes Assisted by Weak Ligand-to-Metal Interactions. A Combined Kinetic and DFT Study. <i>Inorganic Chemistry</i> , 2011, 50, 2224-2239. | 1.9 | 14 |
| 5182 | The Taxadiene-Forming Carbocation Cascade. <i>Journal of the American Chemical Society</i> , 2011, 133, 18249-18256. | 6.6 | 49 |
| 5183 | Mechanisms of Ion-Beam Modification of Terthiophene Oligomers from Atomistic Simulations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23936-23945. | 1.5 | 6 |
| 5184 | Thickness, Surface Morphology, and Optical Properties of Porphyrin Multilayer Thin Films Assembled on Si(100) Using Copper(I)-Catalyzed Azide-Alkyne Cycloaddition. <i>Langmuir</i> , 2011, 27, 4613-4622. | 1.6 | 38 |
| 5185 | Charge Delocalization and Enhanced Acidity in Tricationic Superelectrophiles. <i>Journal of the American Chemical Society</i> , 2011, 133, 13169-13175. | 6.6 | 47 |
| 5186 | Bulk Synthesis and Structure of a Microcrystalline Allotrope of Germanium (<i>m-allo</i> -Ge). <i>Chemistry of Materials</i> , 2011, 23, 4578-4586. | 3.2 | 38 |
| 5187 | Computational Studies of Reactions of Insertion of Rhodium(I) and Iridium(I) into N≡C-H, N≡C-CH ₃ , and NCH ₂ -H Bonds of the Diarylamine-Based PNP Pincer Ligands. <i>Organometallics</i> , 2011, 30, 2972-2979. | 1.1 | 12 |
| 5188 | Synthetic and structural studies on new diiron azadithiolate (ADT)-type model compounds for active site of [FeFe]hydrogenases. <i>Dalton Transactions</i> , 2011, 40, 837-846. | 1.6 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5189 | Theoretical study on intramolecular allene-diene cycloadditions catalyzed by PtCl ₂ and Au(I) complexes. <i>Dalton Transactions</i> , 2011, 40, 11095. | 1.6 | 19 |
| 5190 | Charge transfer in porphyrin-calixarene complexes: ultrafast kinetics, cyclic voltammetry, and DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6947. | 1.3 | 19 |
| 5191 | Electrochemical and spectrophotometrical investigation of the electron-accepting strength of organic superelectrophiles: X-ray structure of their charge transfer complexes with tetrathiafulvalene. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2857-2869. | 1.3 | 13 |
| 5192 | Relativistic effects in a phosphorescent Ir(III) complex. <i>Physical Review B</i> , 2011, 83, . | 1.1 | 39 |
| 5193 | Reaction-Induced Magnetic Transition in Mn ₂ Dimers. <i>Journal of Physical Chemistry A</i> , 2011, 115, 549-555. | 1.1 | 11 |
| 5194 | The Fragmentation-Recombination Mechanism of the Enzyme Glutamate Mutase Studied by QM/MM Simulations. <i>Journal of the American Chemical Society</i> , 2011, 133, 10195-10203. | 6.6 | 32 |
| 5195 | From Structure to Function: Characterization of Cu(I) Adducts in Leveler Additives by DFT Calculations. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 3081-3084. | 2.1 | 9 |
| 5196 | Targeting Intermediates of [FeFe]-Hydrogenase by CO and CN Vibrational Signatures. <i>Inorganic Chemistry</i> , 2011, 50, 3888-3900. | 1.9 | 51 |
| 5197 | Calculation of isotropic Compton profiles with Gaussian basis sets. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5630. | 1.3 | 16 |
| 5198 | trans-Fell(H) ₂ (diphosphine)(diamine) complexes as alternative catalysts for the asymmetric hydrogenation of ketones? A DFT study. <i>Dalton Transactions</i> , 2011, 40, 402-412. | 1.6 | 28 |
| 5199 | Structure and pulsed EPR characterization of N,N-bis(5-tert-butylsalicylidene)-1,2-cyclohexanediamino-vanadium(IV) oxide and its adducts with propylene oxide. <i>Dalton Transactions</i> , 2011, 40, 7454. | 1.6 | 10 |
| 5200 | Cyclopropenylidene carbene ligands in palladium catalysed coupling reactions: carbene ligand rotation and application to the Stille reaction. <i>Dalton Transactions</i> , 2011, 40, 5316. | 1.6 | 15 |
| 5201 | Étude DFT (à base de la théorie fonctionnelle de la densité) des réactions d'addition de l'ozone sur les doubles liaisons des terpènes : limonène, β -phellandrène et terpinolène. <i>Canadian Journal of Chemistry</i> , 2011, 89, 703-708. | 0.6 | 3 |
| 5202 | Free energy of reaction by density functional theory: oxidative addition of ammonia by an iridium complex with PCP pincer ligands. <i>Catalysis Science and Technology</i> , 2011, 1, 1526. | 2.1 | 45 |
| 5203 | A DFT study of IRMOF-3 catalysed Knoevenagel condensation. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 15995. | 1.3 | 29 |
| 5204 | New polycyclic borazine species. <i>Chemical Communications</i> , 2011, 47, 3748. | 2.2 | 25 |
| 5205 | The mixed cyanide halide Au(I) complexes, [XAuCN] ⁺ (X = F, Cl, Br, and I): evolution from ionic to covalent bonding. <i>Chemical Science</i> , 2011, 2, 2101. | 3.7 | 41 |
| 5206 | Electronic spectroscopy of UO ₂ ²⁺ , NUO ⁺ and NUN: an evaluation of time-dependent density functional theory for actinides. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6249. | 1.3 | 77 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5207 | Synthesis and characterization of axial heterojunction inorganic-organic semiconductor nanowire arrays. Dalton Transactions, 2011, 40, 10804. | 1.6 | 28 |
| 5208 | Theoretical simulation of the spectroscopy and dynamics of a red copper protein. Faraday Discussions, 2011, 148, 55-70. | 1.6 | 15 |
| 5209 | Tuning the Laplaza-Cummins 3-coordinate M[N(R)Ph] ₃ catalyst to activate and cleave CO ₂ . Dalton Transactions, 2011, 40, 5569. | 1.6 | 12 |
| 5210 | Photophysical and quantum chemical study on a J-aggregate forming perylene bisimide monomer. Physical Chemistry Chemical Physics, 2011, 13, 17649. | 1.3 | 42 |
| 5211 | New insights on the mechanism of oxidation of d-galacturonic acid by hypervalent chromium. Dalton Transactions, 2011, 40, 7033. | 1.6 | 8 |
| 5212 | Merging the chemistry of electron-rich olefins with imidazolium ionic liquids: radicals and hydrogen-atom adducts. Chemical Science, 2011, 2, 2173. | 3.7 | 17 |
| 5213 | Activation of P ₄ by U(η -5-C ₅ Me ₅)(η -8-C ₈ H ₆ (SiPr ₃) ₂ -1,4)(THF); the X-ray structure of [U(η -5-C ₅ Me ₅)(η -8-C ₈ H ₆ (SiPr ₃) ₂ -1,4)] ₂ (η -1,4- η -2-P ₄). New Journal of Chemistry, 2011, 35, 2022. | 1.4 | 47 |
| 5214 | EPR parameters of amino acid radicals in <i>P. eryngii</i> versatile peroxidase and its W164Y variant computed at the QM/MM level. Physical Chemistry Chemical Physics, 2011, 13, 5078. | 1.3 | 30 |
| 5215 | Assessment of an effective quasirelativistic methodology designed to study astatine chemistry in aqueous solution. Physical Chemistry Chemical Physics, 2011, 13, 14984. | 1.3 | 56 |
| 5216 | Ionization potentials of adenine along the internal conversion pathways. Physical Chemistry Chemical Physics, 2011, 13, 15492. | 1.3 | 28 |
| 5217 | Reductive coupling of carbon monoxide by U(III) complexes—a computational study. Dalton Transactions, 2011, 40, 11080. | 1.6 | 22 |
| 5218 | Achieving C–N bond cleavage in dinuclear metal cyanide complexes. Dalton Transactions, 2011, 40, 7327. | 1.6 | 11 |
| 5219 | 4-Component relativistic magnetically induced current density using London atomic orbitals. Physical Chemistry Chemical Physics, 2011, 13, 20682. | 1.3 | 33 |
| 5220 | Preparation, solid state characterization, and single crystal structure analysis of N-(4-(6-(4-(trifluoromethyl)phenyl)pyrimidin-4-yloxy)benzo[d]thiazol-2-yl)acetamide crystal forms. CrystEngComm, 2011, 13, 1170-1180. | 1.3 | 3 |
| 5221 | Analysis of parity violation in chiral molecules. Physical Chemistry Chemical Physics, 2011, 13, 864-876. | 1.3 | 45 |
| 5222 | Synthesis, characterization and coordination properties of bis(alkyl)selenosalen ligands. Dalton Transactions, 2011, 40, 6684. | 1.6 | 15 |
| 5223 | Low temperature kinetics, crossed beam dynamics and theoretical studies of the reaction S(1D) + CH ₄ and low temperature kinetics of S(1D) + C ₂ H ₂ . Physical Chemistry Chemical Physics, 2011, 13, 8485. | 1.3 | 31 |
| 5224 | A first principles study of water oxidation catalyzed by a tetraruthenium-oxo core embedded in polyoxometalate ligands. Physical Chemistry Chemical Physics, 2011, 13, 7666. | 1.3 | 31 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5225 | Silene equivalents through the rhodium-catalysed reactions of β -hypersilyl diazoesters: a computational and experimental study. <i>Chemical Science</i> , 2011, 2, 2367. | 3.7 | 9 |
| 5226 | Dissociative double photoionization of benzene molecules in the 26–33 eV energy range. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 8245. | 1.3 | 41 |
| 5227 | Picosecond X-ray absorption measurements of the ligand substitution dynamics of Fe(CO) ₅ in ethanol. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5590. | 1.3 | 35 |
| 5228 | A theoretical study of pure and mixed caesium clusters and cluster ions, Cs _n HmO _{0/+n} , n = 5: geometry, energetics and photofragmentation. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14973. | 1.3 | 1 |
| 5229 | Theoretical study on the rearrangement of metallabenzenes to cyclopentadienyl complexes. <i>Dalton Transactions</i> , 2011, 40, 11315. | 1.6 | 32 |
| 5230 | How or not to calculate Ni(II) Werner-type complexes: evaluation of quantum chemical methods. <i>Journal of Coordination Chemistry</i> , 2011, 64, 18-29. | 0.8 | 6 |
| 5231 | Orbital Density Reconstruction for Molecules. <i>Physical Review Letters</i> , 2011, 107, 193002. | 2.9 | 78 |
| 5232 | Solvent-Assisted Naked Eye Sensing of Hg ²⁺ by a Chemoreceptor Derived from Diazocoupling of Sulfathiazole with Diethyl Malonate. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2011, 186, 1820-1834. | 0.8 | 3 |
| 5233 | On the Unexpected Stability of the Dianion of Perylene Diimide in Water—A Computational Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2047-2056. | 1.1 | 49 |
| 5234 | Unraveling the Mechanism of Cascade Reactions of Zincke Aldehydes. <i>Journal of the American Chemical Society</i> , 2011, 133, 3895-3905. | 6.6 | 88 |
| 5235 | Platinum(II) Complexes with Tetradentate Dianionic (O [−]) ₂ C [−] (S [−]) ₂ O-Ligands. <i>Organometallics</i> , 2011, 30, 2980-2985. | 1.1 | 23 |
| 5236 | Highly Twisted Triarylamines for Photoinduced Intramolecular Charge Transfer. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8361-8368. | 1.1 | 20 |
| 5237 | A Stable Aminothioketyl Radical in the Gas Phase. <i>Journal of the American Chemical Society</i> , 2011, 133, 10290-10301. | 6.6 | 1 |
| 5238 | Application of the Quantum Cluster Equilibrium (QCE) Model for the Liquid Phase of Primary Alcohols Using B3LYP and B3LYP-D DFT Methods. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3936-3941. | 1.2 | 30 |
| 5239 | The Need for Enzymatic Steering in Abietic Acid Biosynthesis: Gas-Phase Chemical Dynamics Simulations of Carbocation Rearrangements on a Bifurcating Potential Energy Surface. <i>Journal of the American Chemical Society</i> , 2011, 133, 8335-8343. | 6.6 | 69 |
| 5240 | Structure and Barrier to Methyl Group Internal Rotation for (CF ₃) ₂ CF ₂ OCH ₃ and Its Isomer <i>n</i> -C ₄ F ₉ OCH ₃ (HFE-7100). <i>Journal of Physical Chemistry A</i> , 2011, 115, 1086-1091. | 1.1 | 13 |
| 5241 | Organic Templated Cuprous Cyanide Open Frameworks Based on Cu ₂ (CN) ₆ Dimer with Strong and Long-Lived Luminescence. <i>Crystal Growth and Design</i> , 2011, 11, 3101-3108. | 1.4 | 29 |
| 5242 | Solution-Processed Organic Solar Cells with Power Conversion Efficiencies of 2.5% using Benzothiadiazole/Imide-Based Acceptors. <i>Chemistry of Materials</i> , 2011, 23, 5484-5490. | 3.2 | 232 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5243 | Definitive Benchmark Study of Ring Current Effects on Amide Proton Chemical Shifts. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2078-2084. | 2.3 | 16 |
| 5244 | Tunable One-, Two-, and Three-Dimensional Self-Assemblies from an Acceptor–Donor Fullerene–N-Dimethylaminoazobenzene Dyad: Interfacial Geometry and Temporal Evolution. <i>Langmuir</i> , 2011, 27, 11017-11025. | 1.6 | 12 |
| 5245 | Environmental Effects on the Lignin Model Monomer, Vanillyl Alcohol, Studied by Raman Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2011, 115, 11470-11480. | 1.2 | 20 |
| 5246 | Mechanisms for the Trimethylaluminum Reaction in Aluminum Oxide Atomic Layer Deposition on Sulfur Passivated Germanium. <i>Journal of Physical Chemistry C</i> , 2011, 115, 17523-17532. | 1.5 | 8 |
| 5247 | Surface and Electronic Properties of Hydrogen Terminated Si [001] Nanowires. <i>Journal of Physical Chemistry C</i> , 2011, 115, 12586-12591. | 1.5 | 6 |
| 5248 | CO Adsorption on Noble Metal Clusters: Local Environment Effects. <i>Journal of Physical Chemistry C</i> , 2011, 115, 5637-5647. | 1.5 | 45 |
| 5249 | Effect of Shuttling Catalyst on the Migration of Hydrogen Adatoms: A Strategy for the Facile Hydrogenation of Graphene. <i>Journal of Physical Chemistry C</i> , 2011, 115, 24696-24701. | 1.5 | 33 |
| 5250 | Probing Ground-to-CT State Electronic Coupling for the System with No Apparent Charge Transfer Absorption Intensity by Ultrafast Visible-Pump/Mid-IR-Probe Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2011, 115, 22557-22562. | 1.5 | 8 |
| 5251 | Main-Chain Boron-Containing Oligophenylenes via Ring-Opening Polymerization of 9-H-9-Borafluorene. <i>Journal of the American Chemical Society</i> , 2011, 133, 4596-4609. | 6.6 | 127 |
| 5252 | Ab initio-based Mercury Oxidation Kinetics via Bromine at Postcombustion Flue Gas Conditions. <i>Energy & Fuels</i> , 2011, 25, 1348-1356. | 2.5 | 30 |
| 5253 | Role of Cation Polarization in holo- and hemi-Directed [Pb(H ₂ O) _n] ²⁺ Complexes and Development of a Pb ²⁺ Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 138-147. | 2.3 | 19 |
| 5254 | Quantum-Cascade Laser-Based Vibrational Circular Dichroism. <i>Journal of the American Chemical Society</i> , 2011, 133, 5704-5707. | 6.6 | 41 |
| 5255 | Comparative Assessment of the Composition and Charge State of Nitrogenase FeMo-Cofactor. <i>Inorganic Chemistry</i> , 2011, 50, 4811-4824. | 1.9 | 73 |
| 5256 | Toward Quantitative Structure–Property Relationships for Charge Transfer Rates of Polycyclic Aromatic Hydrocarbons. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2549-2555. | 2.3 | 37 |
| 5257 | Interactions of Phosphororganic Agents with Water and Components of Polyelectrolyte Membranes. <i>Journal of Physical Chemistry B</i> , 2011, 115, 13617-13623. | 1.2 | 23 |
| 5258 | The Lithium–Thiophene Riddle Revisited. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11734-11739. | 1.1 | 21 |
| 5259 | Investigating Inner-Sphere Reorganization via Secondary Kinetic Isotope Effects in the C–H Cleavage Reaction Catalyzed by Soybean Lipoxygenase: Tunneling in the Substrate Backbone as Well as the Transferred Hydrogen. <i>Journal of the American Chemical Society</i> , 2011, 133, 430-439. | 6.6 | 35 |
| 5260 | Synthesis and Structure of Ruthenium(IV) Complexes Featuring N-Heterocyclic Ligands with an N–H Group as the Hydrogen-Bond Donor: Hydrogen Interactions in Solution and in the Solid State. <i>Inorganic Chemistry</i> , 2011, 50, 4868-4881. | 1.9 | 23 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5261 | Theoretical Study of Pt(PR ₃) ₂ (AlCl ₃) (R = H, Me, Ph, or Cy) Including an Unsupported Bond between Transition Metal and Non-transition Metal Elements: Geometry, Bond Strength, and Prediction. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8520-8527. | 1.1 | 9 |
| 5262 | Electronic Structures of Group 9 Metallocorroles with Axial Ammines. <i>Inorganic Chemistry</i> , 2011, 50, 764-770. | 1.9 | 18 |
| 5263 | Edge- versus Vertex-Inversion at Trigonal Pyramidal Ge(II) Centers—A New Aromatic Anchimerically Assisted Edge-Inversion Mechanism. <i>Inorganic Chemistry</i> , 2011, 50, 3651-3661. | 1.9 | 11 |
| 5264 | Solvation Effects on Electronic Transitions: Exploring the Performance of Advanced Solvent Potentials in Polarizable Embedding Calculations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2209-2217. | 2.3 | 75 |
| 5265 | Coarse-Grained Molecular Dynamics Simulations of the Sphere to Rod Transition in Surfactant Micelles. <i>Langmuir</i> , 2011, 27, 6628-6638. | 1.6 | 130 |
| 5266 | Simulations of Solid-State Vibrational Circular Dichroism Spectroscopy of (<i>S</i>)-Alternarolactam by Using Fragmentation Quantum Chemical Calculations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2801-2813. | 1.2 | 37 |
| 5267 | On the Efficiency of Algorithms for Solving Hartree-Fock and Kohn-Sham Response Equations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1610-1630. | 2.3 | 64 |
| 5268 | Development of Polarizable Models for Molecular Mechanical Calculations II: Induced Dipole Models Significantly Improve Accuracy of Intermolecular Interaction Energies. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3100-3111. | 1.2 | 116 |
| 5269 | Charge-Transfer-Like $\pi\pi^*$ Excitations in Time-Dependent Density Functional Theory: A Conundrum and Its Solution. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2408-2415. | 2.3 | 221 |
| 5270 | Aminophenylnitronylnitroxides: Highly Networked Hydrogen-Bond Assembly in Organic Radical Materials. <i>Chemistry of Materials</i> , 2011, 23, 4844-4856. | 3.2 | 9 |
| 5271 | Behavior of Ag ₃ Clusters Inside a Nanometer-Sized Space of ZSM-5 Zeolite. <i>Inorganic Chemistry</i> , 2011, 50, 6533-6542. | 1.9 | 24 |
| 5272 | Evidence for Side-Chain π -Delocalization in a Planar Substituted Benzene: An Experimental and Theoretical Charge Density Study on 2,5-Dimethoxybenzaldehyde Thiosemicarbazone. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12512-12522. | 1.1 | 16 |
| 5273 | Formation of Gallaoxetanes: C=O Activation of 1,2-Epoxybutane by Ground-State Ga Atoms. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11841-11851. | 1.1 | 2 |
| 5274 | Racemization Mechanisms and Electronic Circular Dichroism of [4]Heterohelicene Dyes: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12025-12033. | 1.1 | 18 |
| 5275 | Coordination of 1,10-Phenanthroline and 2,2'-Bipyridine to Li ⁺ in Different Ionic Liquids. How Innocent Are Ionic Liquids?. <i>Inorganic Chemistry</i> , 2011, 50, 6685-6695. | 1.9 | 23 |
| 5276 | Raman Optical Activity Spectra and Conformational Elucidation of Chiral Drugs. The Case of the Antiangiogenic Aeroplysinin-1. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2752-2755. | 1.1 | 22 |
| 5277 | From Inert to Explosive, The Hydrolytic Reactivity of R ¹ NSO Compounds Understood: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 3095-3105. | 1.1 | 9 |
| 5278 | Structure and Gas Sorption Behavior of a New Three Dimensional Porous Magnesium Formate. <i>Inorganic Chemistry</i> , 2011, 50, 1392-1401. | 1.9 | 39 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5279 | Molecular Modeling of Organophosphorous Agents and Their Aqueous Solutions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5201-5209. | 1.1 | 22 |
| 5280 | A Unique Chlorine-Methyl Exchange Reaction upon Treatment of Dichloroorganogallium Compounds, RGaCl_2 , with the Bulky Alkyl lithium Derivative $\text{LiC}(\text{SiMe}_3)_3$. <i>Organometallics</i> , 2011, 30, 3075-3082. | 1.1 | 15 |
| 5281 | Experimental and Theoretical Studies of the Photophysical Properties of 2- and 2,7-Functionalized Pyrene Derivatives. <i>Journal of the American Chemical Society</i> , 2011, 133, 13349-13362. | 6.6 | 284 |
| 5282 | Adsorption of C_2H Radical on Cobalt Clusters: Anion Photoelectron Spectroscopy and Density Functional Calculations. <i>Journal of Physical Chemistry A</i> , 2011, 115, 182-186. | 1.1 | 12 |
| 5283 | Theoretical Study of O-O Single Bond Formation in the Oxidation of Water by the Ruthenium Blue Dimer. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8003-8016. | 1.1 | 46 |
| 5284 | Assembly and Characterization of Well-Defined High-Molecular-Weight Poly(<i>p</i> -phenylene) Polymer Brushes. <i>Chemistry of Materials</i> , 2011, 23, 4367-4374. | 3.2 | 12 |
| 5285 | Intraligand Hydrophobic Interactions Rationalize Drug Affinities for Peptidyl Prolyl Cis-Trans Isomerase Protein. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6193-6201. | 1.2 | 11 |
| 5286 | On the Role of London Dispersion Forces in Biomolecular Structure Determination. <i>Journal of Physical Chemistry B</i> , 2011, 115, 8038-8046. | 1.2 | 41 |
| 5287 | Theoretical Investigation for the Cycle Reaction of N_2O ($x=1$) with CO ($x=1$) Catalyzed by IrO_n ($n=1$). <i>Journal of Physical Chemistry A</i> , 2011, 115, 11023-11032. | 1.1 | 13 |
| 5288 | Computational Insight into the Carbenic Character of Nitrilimines from a Reactivity Perspective. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13694-13705. | 1.1 | 10 |
| 5289 | Effect of Solvation on the Oxygen Reduction Reaction on Pt Catalyst. <i>Journal of Physical Chemistry C</i> , 2011, 115, 7377-7391. | 1.5 | 15 |
| 5290 | $\text{RhCl}(\text{PPh}_3)_3$ -Catalyzed Intramolecular Cycloaddition of Enediyne: The Nature of the Tether and Substituents Controls the Reaction Mechanism. <i>Organometallics</i> , 2011, 30, 3151-3159. | 1.1 | 22 |
| 5291 | Covalency in the 4f Shell of tris-Cyclopentadienyl Ytterbium (YbCp_3)—A Spectroscopic Evaluation. <i>Journal of the American Chemical Society</i> , 2011, 133, 20644-20660. | 6.6 | 56 |
| 5292 | Kinetics and Mechanisms of the Allyl + Allyl and Allyl + Propargyl Recombination Reactions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7610-7624. | 1.1 | 39 |
| 5293 | Non-Innocent Ligand Behavior of a Bimetallic Ni Schiff-Base Complex Containing a Bridging Catecholate. <i>Inorganic Chemistry</i> , 2011, 50, 6746-6755. | 1.9 | 44 |
| 5294 | Structural, Cohesive, Electronic, and Aromatic Properties of Selected Fully and Partially Hydrogenated Carbon Fullerenes. <i>Journal of Physical Chemistry C</i> , 2011, 115, 14507-14516. | 1.5 | 19 |
| 5295 | Tailoring the Cu(100) Work Function by Substituted Benzenethiolate Self-Assembled Monolayers. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7234-7241. | 1.1 | 49 |
| 5296 | Carbon-Bromine Bond Formation through a Nickel-Centered Spin-Crossing Mechanism. <i>Organometallics</i> , 2011, 30, 6365-6371. | 1.1 | 19 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5297 | Thermal Decomposition of 2-Butanol as a Potential Nonfossil Fuel: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2837-2846. | 1.1 | 36 |
| 5298 | Reversible Reductive Dimerization of Diiron η^4 -Vinyl Complex via C-C Coupling: Characterization and Reactivity of the Intermediate Radical Species. <i>Organometallics</i> , 2011, 30, 4115-4122. | 1.1 | 19 |
| 5299 | Electron Affinity of Al ₁₃ : A Correlated Electronic Structure Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 899-903. | 1.1 | 18 |
| 5300 | Visualizing Halogen Bonds in Planar Supramolecular Systems. <i>Journal of Physical Chemistry C</i> , 2011, 115, 2297-2301. | 1.5 | 66 |
| 5301 | Computational Mechanistic Studies Addressed to the Transamination Reaction Present in All Pyridoxal 5'-Phosphate-Requiring Enzymes. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1356-1368. | 2.3 | 46 |
| 5302 | Reactivity and Selectivity of Organotin Reagents in Allylation and Arylation: Nucleophilicity Parameter as a Guide. <i>Organometallics</i> , 2011, 30, 3257-3269. | 1.1 | 22 |
| 5303 | Theoretical Studies on Thermochemistry for Conversion of 5-Chloromethylfurfural into Valuable Chemicals. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13628-13641. | 1.1 | 25 |
| 5304 | Computational Study of Bond Dissociation Enthalpies for a Large Range of Native and Modified Lignins. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2846-2852. | 2.1 | 318 |
| 5305 | Concerted or Stepwise Mechanism? CASPT2 and LC-TDDFT Study of the Excited-State Double Proton Transfer in the 7-Azaindole Dimer. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1006-1015. | 2.3 | 49 |
| 5306 | Redox and Photoisomerization Switching the Second-Order Nonlinear Optical Properties of a Tetrathiafulvalene Derivative Across Six States: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23946-23954. | 1.5 | 83 |
| 5307 | Ab Initio Study on Triplet Excitation Energy Transfer in Photosynthetic Light-Harvesting Complexes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4092-4100. | 1.1 | 30 |
| 5308 | Why Are [P(C6H5)4] ⁺ N3 ⁻ and [As(C6H5)4] ⁺ N3 ⁻ Ionic Salts and Sb(C6H5)4N3 and Bi(C6H5)4N3 Covalent Solids? A Theoretical Study Provides an Unexpected Answer. <i>Inorganic Chemistry</i> , 2011, 50, 3752-3756. | 1.9 | 16 |
| 5309 | Quantifying Asymmetry in Concerted Reactions: Solvents Effect on a Diels-Alder Cycloaddition. <i>Journal of Organic Chemistry</i> , 2011, 76, 4973-4979. | 1.7 | 13 |
| 5310 | Rational Construction of 3D Pillared Metal-Organic Frameworks: Synthesis, Structures, and Hydrogen Adsorption Properties. <i>Inorganic Chemistry</i> , 2011, 50, 7555-7562. | 1.9 | 112 |
| 5311 | Assignment of the Photoelectron Spectra of FeS ₃ by Density Functional Theory, CASPT2, and RCCSD(T) Calculations. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13956-13964. | 1.1 | 20 |
| 5312 | Endohedral Beryllium Atoms in Ten-Vertex Germanium Clusters: Effect of a Small Interstitial Atom on the Cluster Geometry. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2847-2852. | 1.1 | 13 |
| 5313 | Partitioning of Higher Multipole Polarizabilities: Numerical Evaluation of Transferability. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13096-13103. | 1.1 | 13 |
| 5314 | Microsolvation of Uracil and Its Conjugate Bases: A DFT Study of the Role of Solvation on Acidity. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5674-5683. | 1.1 | 21 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5315 | Revisiting the Aufbau Reaction with Acetylene: Further Insights from Experiment and Theory. <i>Organometallics</i> , 2011, 30, 1569-1576. | 1.1 | 10 |
| 5316 | Near-Infrared-Emitting Phthalocyanines. A Combined Experimental and Density Functional Theory Study of the Structural, Optical, and Photophysical Properties of Pd(II) and Pt(II) β -Butoxyphthalocyanines. <i>Inorganic Chemistry</i> , 2011, 50, 1135-1149. | 1.9 | 46 |
| 5317 | ^{15}N Solid-State NMR as a Probe of Flavin H-Bonding. <i>Journal of Physical Chemistry B</i> , 2011, 115, 7788-7798. | 1.2 | 20 |
| 5318 | Reactions of Copper(II)-Phenol Systems with O_2 : Models for TPQ Biosynthesis in Copper Amine Oxidases. <i>Inorganic Chemistry</i> , 2011, 50, 1633-1647. | 1.9 | 26 |
| 5319 | Organoactinides Promote the Dimerization of Aldehydes: Scope, Kinetics, Thermodynamics, and Calculation Studies. <i>Journal of the American Chemical Society</i> , 2011, 133, 1341-1356. | 6.6 | 66 |
| 5320 | Theoretical Study on the Formation of Silacyclopropene from Acylsilane and Acetylene via Silene-to-Silylene Rearrangement. <i>Organometallics</i> , 2011, 30, 3160-3167. | 1.1 | 10 |
| 5321 | How Does the Nickel Pincer Complex Catalyze the Conversion of CO_2 to a Methanol Derivative? A Computational Mechanistic Study. <i>Inorganic Chemistry</i> , 2011, 50, 3816-3825. | 1.9 | 159 |
| 5322 | Molybdenum-Catalyzed Transformation of Molecular Dinitrogen into Silylamine: Experimental and DFT Study on the Remarkable Role of Ferrocenyldiphosphine Ligands. <i>Journal of the American Chemical Society</i> , 2011, 133, 3498-3506. | 6.6 | 148 |
| 5323 | A Step beyond the Feltham-Enemark Notation: Spectroscopic and Correlated <i>ab Initio</i> Computational Support for an Antiferromagnetically Coupled $\text{M(II)}\text{-(NO)}^{\sim}$ Description of $\text{Tp}^*\text{M(NO)}$ ($\text{M} = \text{Co, Ni}$). <i>Journal of the American Chemical Society</i> , 2011, 133, 18785-18801. | 6.6 | 89 |
| 5324 | Catalytic Mechanism of Cytochrome P450 for $5\text{-}\beta$ -Hydroxylation of Nicotine: Fundamental Reaction Pathways and Stereoselectivity. <i>Journal of the American Chemical Society</i> , 2011, 133, 7416-7427. | 6.6 | 110 |
| 5325 | Mechanism and Kinetics of the Reaction $\text{NO}_3 + \text{C}_2\text{H}_4$. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4894-4901. | 1.1 | 15 |
| 5326 | Quantum Chemical Research on Structures, Linear and Nonlinear Optical Properties of the $\text{Li}^+\text{-Acenes Salt}$ ($n = 1, 2, 3, \text{ and } 4$). <i>Journal of Physical Chemistry A</i> , 2011, 115, 2035-2040. | 1.1 | 70 |
| 5327 | Modeling the Deposition of Metal Atoms on a p-Type Organometallic Conductor: Implications for Stability and Electron Transfer. <i>Journal of Physical Chemistry C</i> , 2011, 115, 5997-6003. | 1.5 | 8 |
| 5328 | Understanding the Effect of Adsorption Geometry over Substrate Selectivity in the Surface-Enhanced Raman Scattering Spectra of Simazine and Atrazine. <i>Journal of Physical Chemistry C</i> , 2011, 115, 4184-4190. | 1.5 | 49 |
| 5329 | Weak Molecular Interactions Studied with Parallel Implementations of the Local Pair Natural Orbital Coupled Pair and Coupled Cluster Methods. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 76-87. | 2.3 | 140 |
| 5330 | Aromatic Macrocyclic Containing Amine and Imine Groups: Intramolecular Charge-Transfer and Multiple Redox Behavior. <i>Journal of Organic Chemistry</i> , 2011, 76, 9504-9506. | 1.7 | 7 |
| 5331 | Dissecting Alkynes: Full Cleavage of Polarized $\text{C}\equiv\text{C}$ Moiety via Sequential Bis-Michael Addition/Retro-Mannich Cascade. <i>Journal of Organic Chemistry</i> , 2011, 76, 7482-7490. | 1.7 | 56 |
| 5332 | Evolution of Properties in Prolate $(\text{GaAs})_n$ Clusters. <i>Journal of Physical Chemistry C</i> , 2011, 115, 97-107. | 1.5 | 30 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5333 | Properties of Carbon Nanotubes: An ab Initio Study Using Large Gaussian Basis Sets and Various DFT Functionals. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8876-8885. | 1.5 | 42 |
| 5334 | Density Functional Study of Hydrogen Bond Formation between Methanol and Organic Molecules Containing Cl, F, NH ₂ , OH, and COOH Functional Groups. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14054-14068. | 1.1 | 19 |
| 5335 | Hydroboration of Disilyne RSiR ₂ SiR ₂ (R =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 667 Td (Si ⁺ Pr[CH(SiMe ₃)] ₃)] Disilenes. <i>Organometallics</i> , 2011, 30, 2044-2050. | 1.1 | 38 |
| 5336 | Understanding Optoelectronic Properties of Cyano-Terminated Oligothiophenes in the Context of Intramolecular Charge Transfer. <i>Journal of Physical Chemistry B</i> , 2011, 115, 10573-10585. | 1.2 | 23 |
| 5337 | Computational Insights into Palladium-Mediated Allylic Substitution Reactions. <i>Topics in Organometallic Chemistry</i> , 2011, , 65-93. | 0.7 | 24 |
| 5338 | Donor-Substituted Diphenylacetylene Derivatives Act as Electron Donors and Acceptors. <i>Journal of Organic Chemistry</i> , 2011, 76, 5628-5635. | 1.7 | 10 |
| 5339 | Modeling interactions between lignocellulose and ionic liquids using DFT-D. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11393. | 1.3 | 112 |
| 5340 | Effects of Solvents, Ligand Aromaticity, and Coordination Sphere on the g Tensor of Anionic o -Semiquinone Radicals Complexed by Mg ²⁺ Ions: DFT Studies. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3172-3184. | 1.2 | 24 |
| 5341 | Photoinduced Rearrangement of Aromatic N -Chloroamides to Chloroaromatic Amides in the Solid State: Inverted N -Occupational Stability of Amidyl Radicals. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7834-7848. | 1.1 | 8 |
| 5342 | TD-DFT Vibronic Couplings in Anthraquinones: From Basis Set and Functional Benchmarks to Applications for Industrial Dyes. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1882-1892. | 2.3 | 113 |
| 5344 | Hydration of Simple Carboxylic Acids from Infrared Spectra of HDO and Theoretical Calculations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4834-4842. | 1.2 | 17 |
| 5345 | Double-hybrid density-functional theory made rigorous. <i>Journal of Chemical Physics</i> , 2011, 134, 064113. | 1.2 | 165 |
| 5346 | Theoretical prediction of new dipole-bound singlet states for anions of interstellar interest. <i>Journal of Chemical Physics</i> , 2011, 134, 154304. | 1.2 | 48 |
| 5347 | Highly enantioselective cascade synthesis of spiropyrazolones. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 6519. | 1.5 | 104 |
| 5348 | Synthesis and characterization of bis-cyclopropanated 1,3,5-tricarbonyl compounds. A combined synthetic, spectroscopic and theoretical study. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 5172. | 1.5 | 11 |
| 5349 | Nuclear magnetic resonance shielding constants and chemical shifts in linear 199Hg compounds: A comparison of three relativistic computational methods. <i>Journal of Chemical Physics</i> , 2011, 135, 044306. | 1.2 | 55 |
| 5350 | Gd ₂ @C ₇₉ N: Isolation, Characterization, and Monoadduct Formation of a Very Stable Heterofullerene with a Magnetic Spin State of $S = 15/2$. <i>Journal of the American Chemical Society</i> , 2011, 133, 9741-9750. | 6.6 | 104 |
| 5351 | Cyclopropylhydroxycarbene. <i>Journal of the American Chemical Society</i> , 2011, 133, 13614-13621. | 6.6 | 59 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5352 | Conformational Enantiomerization and Estrogen Receptor $\hat{\pm}$ Binding of Anti-Cancer Drug Tamoxifen and Its Derivatives. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 306-314. | 2.5 | 8 |
| 5353 | DFT Study of Thermal 1,3-Dipolar Cycloaddition Reactions between Alkynyl Metal(0) Fischer Carbene Complexes and 3-H-1,2-Dithiole-3-thione Derivatives. <i>Organometallics</i> , 2011, 30, 466-476. | 1.1 | 38 |
| 5354 | Accurate Band Gaps for Semiconductors from Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 212-217. | 2.1 | 444 |
| 5355 | The solid-state organization of $\hat{\epsilon}$ -self-doped $\hat{\epsilon}$ ™ PPV oligomers. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18516. | 1.3 | 3 |
| 5356 | Amylose $\hat{\epsilon}$ “Vanillin Complexation Assessed by a Joint Experimental and Theoretical Analysis. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23315-23322. | 1.5 | 19 |
| 5358 | Parameterization of a B3LYP Specific Correction for Noncovalent Interactions and Basis Set Superposition Error on a Gigantic Data Set of CCSD(T) Quality Noncovalent Interaction Energies. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 658-668. | 2.3 | 73 |
| 5359 | Separating Electrophilicity and Lewis Acidity: The Synthesis, Characterization, and Electrochemistry of the Electron Deficient <i>Tris</i> (aryl)boranes $B(C_6F_5)_3$ (C_6Cl_5) _n ($n = 1-3$). <i>Journal of the American Chemical Society</i> , 2011, 133, 14727-14740. | 6.6 | 153 |
| 5360 | Oscillator Strength: How Does TDDFT Compare to EOM-CCSD?. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 456-466. | 2.3 | 123 |
| 5361 | Noncollinear Spins Provide a Self-Consistent Treatment of the Low-Spin State of a Biomimetic Oxomanganese Synthetic Trimer Inspired by the Oxygen Evolving Complex of Photosystem II. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2629-2633. | 2.1 | 29 |
| 5362 | Pople Style Basis Sets for the Calculation of NMR Spin $\hat{\epsilon}$ “Spin Coupling Constants: the 6-31G-J and 6-311G-J Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4070-4076. | 2.3 | 52 |
| 5363 | Understanding Conjugation and Hyperconjugation from Electronic Delocalization Measures. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13104-13113. | 1.1 | 30 |
| 5364 | Accuracy of Density Functionals in the Prediction of Electronic Proton Affinities of Amino Acid Side Chains. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3898-3908. | 2.3 | 45 |
| 5365 | The reactivity of endohedral fullerenes. What can be learnt from computational studies?. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 3585-3603. | 1.3 | 128 |
| 5366 | A theoretical study of a ZnO graphene analogue: adsorption on Ag(111) and hydrogen transport. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 334215. | 0.7 | 5 |
| 5367 | Chameleonic Reactivity of Vicinal Diazonium Salt of Acetylenyl-9,10-anthraquinones: Synthetic Application toward Two Heterocyclic Targets. <i>Journal of Organic Chemistry</i> , 2011, 76, 8737-8748. | 1.7 | 21 |
| 5368 | Relativistic Four-Component DFT Calculations of ¹ H NMR Chemical Shifts in Transition-Metal Hydride Complexes: Unusual High-Field Shifts Beyond the Buckingham $\hat{\epsilon}$ “Stephens Model. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5654-5659. | 1.1 | 120 |
| 5369 | Benzothiazoles with Tunable Electron-Withdrawing Strength and Reverse Polarity: A Route to Triphenylamine-Based Chromophores with Enhanced Two-Photon Absorption. <i>Journal of Organic Chemistry</i> , 2011, 76, 8726-8736. | 1.7 | 138 |
| 5370 | Theoretical Insights into Heme-Catalyzed Oxidation of Cyclohexane to Adipic Acid. <i>Inorganic Chemistry</i> , 2011, 50, 1194-1202. | 1.9 | 31 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 5371 | Benchmarking Semiempirical Methods for Thermochemistry, Kinetics, and Noncovalent Interactions: OMx Methods Are Almost As Accurate and Robust As DFT-GGA Methods for Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2929-2936. | 2.3 | 89 |
| 5372 | Protein-Ligand Interaction Energies with Dispersion Corrected Density Functional Theory and High-Level Wave Function Based Methods. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11210-11220. | 1.1 | 78 |
| 5373 | On the Mechanism of the Copper-Mediated C-S Bond Formation in the Intramolecular Disproportionation of Imine Disulfides. <i>Inorganic Chemistry</i> , 2011, 50, 9968-9979. | 1.9 | 16 |
| 5374 | Stoichiometric and Oxygen-Rich M_2O_n and M_2O_n ($M = Nb, Ta; n = 5-7$) Clusters: Molecular Models for Oxygen Radicals, Diradicals, and Superoxides. <i>Journal of the American Chemical Society</i> , 2011, 133, 3085-3094. | 6.6 | 49 |
| 5375 | Charge-transfer and the hydrogen bond: Spectroscopic and structural implications from electronic structure calculations. <i>Faraday Discussions</i> , 2011, 150, 345. | 1.6 | 59 |
| 5376 | Role of Many-Body Effects in Describing Low-Lying Excited States of π -Conjugated Chromophores: High-Level Equation-of-Motion Coupled-Cluster Studies of Fused Porphyrin Systems. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2200-2208. | 2.3 | 22 |
| 5377 | Experimental and Computational Thermochemical Study of N-Benzylalanines. <i>Journal of Physical Chemistry B</i> , 2011, 115, 9401-9409. | 1.2 | 10 |
| 5378 | Nitrogenase Structure and Function Relationships by Density Functional Theory. <i>Methods in Molecular Biology</i> , 2011, 766, 267-291. | 0.4 | 5 |
| 5379 | N,N -Bis(diphenylphosphino)diaminophenylphosphine Ligands for Chromium-Catalyzed Selective Ethylene Oligomerization Reactions. <i>Organometallics</i> , 2011, 30, 935-941. | 1.1 | 39 |
| 5380 | Theoretical Study of the Structural Properties of Plutonium(IV) and (VI) Complexes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14110-14119. | 1.1 | 35 |
| 5381 | How do electron localization functions describe π -electron delocalization?. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20584. | 1.3 | 99 |
| 5382 | Theoretical investigations into the enantiomeric and racemic forms of \pm -(trifluoromethyl)lactic acid. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 811-817. | 1.3 | 17 |
| 5383 | Endocyclic Cleavage in Glycosides with 2,3- <i>trans</i> -Cyclic Protecting Groups. <i>Journal of the American Chemical Society</i> , 2011, 133, 5610-5619. | 6.6 | 62 |
| 5384 | Solvation Structure and Dynamics of Ni^{2+} (aq) from First Principles. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2937-2946. | 2.3 | 11 |
| 5385 | A Sulfonium Cation Intermediate in the Mechanism of Methionine Sulfoxide Reductase B: A DFT Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 9202-9212. | 1.2 | 12 |
| 5386 | Ammonia Activation by λ^3 -Alkylidyne Fragments Supported on a Titanium Molecular Oxide Model. <i>Inorganic Chemistry</i> , 2011, 50, 6269-6279. | 1.9 | 39 |
| 5387 | Mechanisms of Reactions of a Lithium Boryl with Organohalides. <i>Organometallics</i> , 2011, 30, 3018-3028. | 1.1 | 40 |
| 5388 | Energy levels, charge injection, charge recombination and dye regeneration dynamics for donor-acceptor π -conjugated organic dyes in mesoscopic TiO ₂ sensitized solar cells. <i>Energy and Environmental Science</i> , 2011, 4, 1820. | 15.6 | 140 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5390 | Nature and strength of C=O interactions involving formyl hydrogen atoms: computational and experimental studies of small aldehydes. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14076. | 1.3 | 83 |
| 5391 | Accurate Dispersion-Corrected Density Functionals for General Chemistry Applications. , 2011, , 1-16. | | 2 |
| 5392 | On the Nature of Lithium Biphenyl in Ethereal Solvents. A Critical Analysis Unifying DFT Calculations, Physicochemical Data in Solution, and a X-ray Structure. <i>Journal of Physical Chemistry B</i> , 2011, 115, 14610-14616. | 1.2 | 15 |
| 5393 | Novel Dinuclear Platinum(II) Complexes Containing Mixed Nitrogen-Sulfur Donor Ligands. <i>Inorganic Chemistry</i> , 2011, 50, 12747-12761. | 1.9 | 22 |
| 5394 | Spin Ground State and Magnetic Properties of Cobalt(II): Relativistic DFT Calculations Guided by EPR Measurements of Bis(2,4-acetylacetonate)cobalt(II)-Based Complexes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2316-2324. | 1.1 | 36 |
| 5395 | Redox Noninnocence of Nitrosoarene Ligands in Transition Metal Complexes. <i>Inorganic Chemistry</i> , 2011, 50, 5763-5776. | 1.9 | 57 |
| 5396 | Intramolecular Hydrogen Bonds: the QTAIM and ELF Characteristics. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10078-10086. | 1.1 | 176 |
| 5397 | Routes of π -Electron Delocalization in 4-Substituted-1,2-benzoquinones. <i>Journal of Organic Chemistry</i> , 2011, 76, 550-556. | 1.7 | 15 |
| 5398 | Surface-Enhanced Raman Scattering on Semiconducting Oxide Nanoparticles: Oxide Nature, Size, Solvent, and pH Effects. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8994-9004. | 1.5 | 79 |
| 5399 | DFT-B3LYP, NPA-, and QTAIM-Based Study of the Physical Properties of [M(II)(H ₂ O) ₂ (15-crown-5)] (M = Mn, Fe, Co, Ni, Cu, Zn) Complexes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5592-5601. | 1.1 | 46 |
| 5400 | Extraordinary Difference in Reactivity of Ozone (OOO) and Sulfur Dioxide (OSO): A Theoretical Study. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2104-2111. | 2.3 | 63 |
| 5401 | Conformational Analysis of 18-Azacrown-6 and Its Bonding with Late First Transition Series Divalent Metals: Insight from DFT Combined with NPA and QTAIM Analyses. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13180-13190. | 1.1 | 33 |
| 5402 | Interatomic Magnetizability: A QTAIM-Based Approach toward Deciphering Magnetic Aromaticity. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12555-12560. | 1.1 | 35 |
| 5403 | A periodic mixed gaussians-plane waves DFT study on simple thiols on Au(111): adsorbate species, surface reconstruction, and thiols functionalization. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 3886. | 1.3 | 32 |
| 5404 | The chemistry of acetone at extreme conditions by density functional molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2011, 134, 064502. | 1.2 | 0 |
| 5405 | Water Oxidation by a Mononuclear Ruthenium Catalyst: Characterization of the Intermediates. <i>Journal of the American Chemical Society</i> , 2011, 133, 14649-14665. | 6.6 | 180 |
| 5406 | Aggregation of Alkyltrimethylammonium Ions at the Cleaved Muscovite Mica-Water Interface: A Monte Carlo Study. <i>Langmuir</i> , 2011, 27, 12968-12976. | 1.6 | 10 |
| 5407 | Solvent-Induced Shift of the Lowest Singlet $\pi \rightarrow \pi^*$ Charge-Transfer Excited State of <i>p</i> -Nitroaniline in Water: An Application of the TDDFT/EFP1 Method. <i>Journal of Physical Chemistry A</i> , 2011, 115, 9801-9809. | 1.1 | 49 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5408 | Revisiting the Effects of Sequence and Structure on the Hydrogen Bonding and π -Stacking Interactions in Nucleic Acids. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12800-12808. | 1.1 | 15 |
| 5409 | A Density Functional Theory Study of the Nef-Isocyanide Reaction: Mechanism, Influence of Parameters and Scope. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10106-10112. | 1.1 | 11 |
| 5410 | Accurate Conformational Energy Differences of Carbohydrates: A Complete Basis Set Extrapolation. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 988-997. | 2.3 | 26 |
| 5411 | Electronic level alignment at a metal-molecule interface from a short-range hybrid functional. <i>Journal of Chemical Physics</i> , 2011, 135, 164706. | 1.2 | 71 |
| 5412 | Using the Outer Coordination Sphere to Tune the Strength of Metal Extractants. <i>Inorganic Chemistry</i> , 2011, 50, 4515-4522. | 1.9 | 37 |
| 5413 | CCSD-PCM: Improving upon the reference reaction field approximation at no cost. <i>Journal of Chemical Physics</i> , 2011, 135, 074113. | 1.2 | 42 |
| 5414 | Bond energy analysis revisited and designed toward a rigorous methodology. <i>Journal of Chemical Physics</i> , 2011, 135, 124105. | 1.2 | 8 |
| 5415 | Performance of Density Functional Theory and Møller-Plesset Second-Order Perturbation Theory for Structural Parameters in Complexes of Ru. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2325-2332. | 2.3 | 131 |
| 5416 | Valence Shell Charge Concentration (VSCC) Evolution: A Tool to Investigate the Transformations within a VSCC Throughout a Chemical Reaction. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12924-12932. | 1.1 | 14 |
| 5417 | Computational Investigation of Selectivity in Suzuki-Miyaura Coupling of Secondary Alkyl Boranes. <i>Organometallics</i> , 2011, 30, 4564-4571. | 1.1 | 15 |
| 5418 | Dispersion Corrections Essential for the Study of Chemical Reactivity in Fullerenes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 3491-3496. | 1.1 | 117 |
| 5419 | π -conjugation and charge polarization in fluorene-dibenzothiophene-S,S-dioxide co-oligomers by Raman spectroscopy and quantum chemistry. <i>Journal of Chemical Physics</i> , 2011, 134, 044520. | 1.2 | 13 |
| 5421 | Computational calculations of pKa values of imidazole in Cu(II) complexes of biological relevance. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 7852. | 1.3 | 55 |
| 5422 | Adsorption and diffusion of water on graphene from first principles. <i>Physical Review B</i> , 2011, 84, . | 1.1 | 218 |
| 5423 | Carbonyl Oxides Reactions from Geraniol-trans-(3,7-dimethylocta-2,6-dien-1-ol), 6-Methyl-5-hepten-2-one, and 6-Hydroxy-4-methyl-4-hexenal Ozonolysis: Kinetics and Mechanisms. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7709-7721. | 1.1 | 6 |
| 5424 | On the Influence of Density Functional Approximations on Some Local Bader's Atoms-in-Molecules Properties. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5505-5515. | 1.1 | 52 |
| 5425 | Ruthenium nitrosyl complexes with 1,4,7-trithiacyclononane and 2,2'-bipyridine (bpy) or 2-phenylazopyridine (pap) coligands. Electronic structure and reactivity aspects. <i>Dalton Transactions</i> , 2011, 40, 12527. | 1.6 | 27 |
| 5426 | Does the concept of Clar's aromatic sextet work for dicationic forms of polycyclic aromatic hydrocarbons?—testing the model against charged systems in singlet and triplet states. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11976-11984. | 1.3 | 25 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5427 | 2-(3,5-Dinitrophenyl)-1,3-dithiane Carbanion: A Benzylic Anion with a Low Energy Triplet State. <i>Journal of the American Chemical Society</i> , 2011, 133, 15553-15558. | 6.6 | 22 |
| 5428 | Spontaneous Dissociation of Xenon Tetroxide: Phase and Structural Changes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7811-7814. | 1.1 | 4 |
| 5429 | DFT Study of Trichloroethene Reaction with Permanganate in Aqueous Solution. <i>Environmental Science & Technology</i> , 2011, 45, 3006-3011. | 4.6 | 29 |
| 5430 | Theoretical Spectroscopy of Astaxanthin in Crustacyanin Proteins: Absorption, Circular Dichroism, and Nuclear Magnetic Resonance. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3216-3225. | 1.2 | 33 |
| 5431 | A rational design strategy for donors in organic solar cells: the conjugated planar molecules possessing anisotropic multibranches and intramolecular charge transfer. <i>Journal of Materials Chemistry</i> , 2011, 21, 11159. | 6.7 | 36 |
| 5432 | A Computationally Efficient and Reliable Bond Order Measure. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4397-4405. | 1.1 | 8 |
| 5433 | Theoretical Study of Pyridoxine (Vitamin B6) Photolysis. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13556-13563. | 1.1 | 12 |
| 5434 | Density Functional Calculation of the Structure and Electronic Properties of Cu_nO_n ($n = 1\text{--}8$) Clusters. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2087-2095. | 1.1 | 39 |
| 5435 | Unexpected size distribution of $\text{Ba}(\text{H}_2\text{O})_n$ clusters: why is the intensity of the $\text{Ba}(\text{H}_2\text{O})_1$ cluster anomalously low?. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13387. | 1.3 | 4 |
| 5436 | Electronic and Magnetic Properties of Chiral Molecules and Supramolecular Architectures. <i>Topics in Current Chemistry</i> , 2011, . . | 4.0 | 16 |
| 5437 | Dithizone and Its Oxidation Products: A DFT, Spectroscopic, and X-ray Structural Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14637-14646. | 1.1 | 29 |
| 5438 | Subshell Fitting of Relativistic Atomic Core Electron Densities for Use in QTAIM Analyses of ECP-Based Wave Functions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12879-12894. | 1.1 | 41 |
| 5439 | Application of Molecular Simulation Techniques to the Study of Factors Affecting the Thin-Film Morphology of Small-Molecule Organic Semiconductors. <i>Chemistry of Materials</i> , 2011, 23, 522-543. | 3.2 | 52 |
| 5440 | Multidecker Bis(benzene)chromium: Opportunities for Design of Rigid and Highly Flexible Molecular Wires. <i>Journal of Physical Chemistry C</i> , 2011, 115, 785-790. | 1.5 | 19 |
| 5441 | Bridging Interactions and Selective Nanoparticle Aggregation Mediated by Monovalent Cations. <i>ACS Nano</i> , 2011, 5, 530-536. | 7.3 | 71 |
| 5442 | DFT Study of Electronic Properties of 3d Metal Complexes of β -Geminal Diethynylethenes (β -DEEs). <i>Organometallics</i> , 2011, 30, 245-250. | 1.1 | 26 |
| 5443 | GPU-Based Implementations of the Noniterative Regularized-CCSD(T) Corrections: Applications to Strongly Correlated Systems. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1316-1327. | 2.3 | 72 |
| 5444 | A new building block for electroactive organic materials? Synthesis, cyclic voltammetry, single crystal X-ray structure, and DFT treatment of a unique boron-based viologen. <i>Chemical Communications</i> , 2011, 47, 9072. | 2.2 | 9 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5445 | Probing the electronic and optical properties of silica-coated quantum dots with first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14476. | 1.3 | 4 |
| 5446 | Implementation of screened hybrid functionals based on the Yukawa potential within the LAPW basis set. <i>Physical Review B</i> , 2011, 83, . | 1.1 | 159 |
| 5447 | New Series of Triply Bridged Dinuclear Cu(II) Compounds: Synthesis, Crystal Structure, Magnetic Properties, and Theoretical Study. <i>Inorganic Chemistry</i> , 2011, 50, 10648-10659. | 1.9 | 31 |
| 5448 | Reaction Mechanism of the Reverse Water-Gas Shift Reaction Using First-Row Middle Transition Metal Catalysts M ($M = Fe, Mn, Co$): A Computational Study. <i>Inorganic Chemistry</i> , 2011, 50, 8782-8789. | 1.9 | 27 |
| 5449 | Observation of Inductive Effects That Cause a Change in the Rate-Determining Step for the Conversion of Rhenium Azides to Imido Complexes. <i>Inorganic Chemistry</i> , 2011, 50, 10505-10514. | 1.9 | 16 |
| 5450 | High-Valent Uranium Alkyls: Evidence for the Formation of $U^{VI}(CH_2)_2SiMe_3$. <i>Journal of the American Chemical Society</i> , 2011, 133, 11732-11743. | 6.6 | 87 |
| 5451 | THE INFRARED SPECTROSCOPY OF POLYCYCLIC AROMATIC HYDROCARBONS WITH FIVE- AND SEVEN-MEMBERED FUSED RING DEFECTS. <i>Astrophysical Journal</i> , 2011, 729, 94. | 1.6 | 24 |
| 5452 | Accuracy of Effective Core Potentials and Basis Sets for Density Functional Calculations, Including Relativistic Effects, As Illustrated by Calculations on Arsenic Compounds. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2766-2779. | 2.3 | 78 |
| 5453 | Calibration of DFT Functionals for the Prediction of ^{57}Fe Mössbauer Spectral Parameters in Iron-Nitrosyl and Iron-Sulfur Complexes: Accurate Geometries Prove Essential. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3232-3247. | 2.3 | 70 |
| 5454 | Excited-State Studies of Polyacenes: A Comparative Picture Using EOMCCSD, CR-EOMCCSD(T), Range-Separated (LR/RT)-TDDFT, TD-PM3, and TD-ZINDO. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3686-3693. | 2.3 | 84 |
| 5455 | Hybrid Quantum and Classical Simulations of the Dihydrofolate Reductase Catalyzed Hydride Transfer Reaction on an Accurate Semi-Empirical Potential Energy Surface. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3420-3437. | 2.3 | 45 |
| 5456 | Magnetic Coupling in Transition-Metal Binuclear Complexes by Spin-Flip Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3523-3531. | 2.3 | 52 |
| 5457 | On the Importance of the Orbital Relaxation in Ground-State Coupled Cluster Calculations in Solution with the Polarizable Continuum Model of Solvation. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4012-4018. | 2.3 | 9 |
| 5458 | On the Origin of the Chiro-Optical Activity in Supramolecular Assemblies: A Quantum Chemical Study of C_3 Octopolar Systems. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3314-3322. | 2.3 | 5 |
| 5459 | OCO and NCO chelated derivatives of heavier group 15 elements. Study on possibility of cyclization reaction via intramolecular ether bond cleavage. <i>Dalton Transactions</i> , 2011, 40, 8922. | 1.6 | 35 |
| 5460 | On the mechanism of water oxidation by a bimetallic manganese catalyst: A density functional study. <i>Dalton Transactions</i> , 2011, 40, 3859. | 1.6 | 44 |
| 5461 | Effects of Peripheral and Axial Substitutions on Electronic Transitions of Tin Naphthalocyanines. <i>Journal of Physical Chemistry A</i> , 2011, 115, 9265-9272. | 1.1 | 11 |
| 5462 | Decorating Diruthenium Compounds with Fractal Dendrons via the Click Reaction. <i>Inorganic Chemistry</i> , 2011, 50, 9345-9353. | 1.9 | 14 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 5463 | Electronic Stabilization of Trigonal Bipyramidal Clusters: the Role of the Sn(II) Ions in $[Pt_5(CO)_5\{Cl_2Sn(\frac{1}{4}OR)SnCl_2\}_3]^{3-}$ (R = H, Me, Et, Pr). <i>Inorganic Chemistry</i> , 2011, 50, 12553-12561. | | 16 |
| 5464 | Electronic Structures and Spectroscopy of the Electron Transfer Series $[Fe(NO)L_2]^{z/l}$ ($z/l = 1+, 0, 1^-, 2^-, 3^-$; L = Dithiolene). <i>Inorganic Chemistry</i> , 2011, 50, 12064-12074. | 1.9 | 28 |
| 5465 | Fluxionality of Hydrogen Ligands in $Fe(H)_2(H)_2(PtPh)_2$. <i>Inorganic Chemistry</i> , 2011, 50, 10740-10747. | 1.9 | 15 |
| 5466 | Isolation and Assessment of the Molecular and Electronic Structures of Azo-Anion-Radical Complexes of Chromium and Molybdenum. Experimental and Theoretical Characterization of Complete Electron-Transfer Series. <i>Inorganic Chemistry</i> , 2011, 50, 9993-10004. | 1.9 | 47 |
| 5467 | Limited Occurrence of <i>Isocloso</i> Deltahedra with 9 to 12 Vertices in Low-Energy Hypoelectronic Diferradicarbaborane Structures. <i>Inorganic Chemistry</i> , 2011, 50, 9571-9577. | 1.9 | 25 |
| 5468 | Mechanistic Investigation of the Ru-Catalyzed Hydroamidation of Terminal Alkynes. <i>Journal of the American Chemical Society</i> , 2011, 133, 7428-7449. | 6.6 | 73 |
| 5469 | Kinetics and Mechanism of S-Nitrosothiol Acid-Catalyzed Hydrolysis: Sulfur Activation Promotes Facile NO ⁺ Release. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3112-3126. | 1.2 | 27 |
| 5470 | Counterion Dynamics in Polyurethane-Carboxylate Ionomers with Ionic Liquid Counterions. <i>Chemistry of Materials</i> , 2011, 23, 1862-1873. | 3.2 | 92 |
| 5471 | Oxazoles revisited: On the nature of binding of benzoxazole and 2-methylbenzoxazole with the zinc and palladium halides. <i>Dalton Transactions</i> , 2011, 40, 1594. | 1.6 | 11 |
| 5472 | Polymorphs of <i>N</i> -[2-(Hydroxymethyl)phenyl]benzamide: Structural Characterization and Analysis of Molecule-Molecule Interactions by Means of Atom-Atom Potentials and DFT. <i>Crystal Growth and Design</i> , 2011, 11, 1431-1436. | 1.4 | 7 |
| 5473 | Structure, dynamics, and solvation in a disordered metal-organic coordination polymer: a multiscale study. <i>Journal of Coordination Chemistry</i> , 2011, 64, 4301-4317. | 0.8 | 5 |
| 5474 | Proton management as a design principle for hydrogenase-inspired catalysts. <i>Energy and Environmental Science</i> , 2011, 4, 3008. | 15.6 | 50 |
| 5475 | An Extension of the Hirshfeld Method to Open Shell Systems Using Fractional Occupations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1328-1335. | 2.3 | 50 |
| 5476 | A DFT comparison of the neutral and cationic Heck pathways. <i>Dalton Transactions</i> , 2011, 40, 11308. | 1.6 | 36 |
| 5477 | Complexation of alkali-metal cations by conformationally rigid, stereoisomeric calix[4]arene crown ethers: A density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2011, 967, 235-242. | 1.1 | 8 |
| 5478 | Electronic, optical and charge transfer properties of $\hat{1}, \hat{1}^{\pm}$ -bis(dithieno[3,2-b:2',3'-d]thiophene) (BDT) and its heteroatom-substituted analogues. <i>Computational and Theoretical Chemistry</i> , 2011, 968, 8-11. | 1.1 | 19 |
| 5479 | Theoretical investigation on the reaction of N ₂ O and CO catalyzed by PtO ⁺ . <i>Computational and Theoretical Chemistry</i> , 2011, 968, 31-38. | 1.1 | 6 |
| 5480 | A DFT/TDDFT study of hydrogen bonding interactions between resorufin anion and water molecules in the excited state. <i>Computational and Theoretical Chemistry</i> , 2011, 970, 6-14. | 1.1 | 10 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5481 | Density functional theory calculations of iodine cluster anions: Structures, chemical bonding nature, and vibrational spectra. <i>Computational and Theoretical Chemistry</i> , 2011, 973, 69-75. | 1.1 | 16 |
| 5482 | Theoretical views on the cycle reaction of $N_2O(1\hat{1}\xi^+)+NH_3(1A1)+O_2$ catalyzed by Fe^+ and utilizing the energy span model to study its kinetic information. <i>Computational and Theoretical Chemistry</i> , 2011, 974, 143-150. | 1.1 | 3 |
| 5483 | Mechanistic insight into the DPPH radical-scavenging activity of hydroxystilbene derivatives. <i>Computational and Theoretical Chemistry</i> , 2011, 974, 159-162. | 1.1 | 3 |
| 5484 | Nano-molecular springs: How high will it jump?. <i>Computational and Theoretical Chemistry</i> , 2011, 977, 55-61. | 1.1 | 1 |
| 5485 | Cooperative effects in regular and bifurcated intramolecular $OH\hat{\alpha}^{\leftarrow}OC$ interactions: A computational study. <i>Computational and Theoretical Chemistry</i> , 2011, 977, 181-187. | 1.1 | 13 |
| 5486 | Inhibition of copper corrosion in sodium chloride solution by the self-assembled monolayer of sodium diethyldithiocarbamate. <i>Corrosion Science</i> , 2011, 53, 1999-2005. | 3.0 | 62 |
| 5487 | The Eltard Reaction: A DFT Study. <i>Inorganic Chemistry</i> , 2011, 50, 5833-5840. | 1.9 | 5 |
| 5488 | Non-redox Oxy-Insertion via Organometallic Baeyer-Villiger Transformations: A Computational Hammett Study of Platinum(II) Complexes. <i>Organometallics</i> , 2011, 30, 3779-3785. | 1.1 | 35 |
| 5489 | Electronic structure of tris(8-hydroxyquinolinato)aluminium(III) revisited using the Heyd-Scuseria-Ernzerhof hybrid functional: Theory and experiments. <i>Physical Review B</i> , 2011, 84, . | 1.1 | 17 |
| 5490 | Comparative study of hybrid functionals applied to structural and electronic properties of semiconductors and insulators. <i>Physical Review B</i> , 2011, 84, . | 1.1 | 67 |
| 5491 | $Ion\hat{\alpha}^{\leftarrow}$ ion and $ion\hat{\alpha}^{\leftarrow}$ solvent interactions in lithium imidazolide electrolytes studied by Raman spectroscopy and DFT models. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11136. | 1.3 | 33 |
| 5492 | Does Compound I Vary Significantly between Isoforms of Cytochrome P450?. <i>Journal of the American Chemical Society</i> , 2011, 133, 15464-15474. | 6.6 | 188 |
| 5493 | Defect-trapped electrons and ferromagnetic exchange in ZnO. <i>Physical Review B</i> , 2011, 84, . | 1.1 | 44 |
| 5494 | N-Heterocyclic Carbene-Amide Rhodium(I) Complexes: Structures, Dynamics, and Catalysis. <i>Organometallics</i> , 2011, 30, 5258-5272. | 1.1 | 66 |
| 5495 | On the gauge invariance of nonperturbative electronic dynamics using the time-dependent Hartree-Fock and time-dependent Kohn-Sham. <i>Journal of Chemical Physics</i> , 2011, 135, 164101. | 1.2 | 41 |
| 5496 | Validation of electronic structure methods for isomerization reactions of large organic molecules. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13683. | 1.3 | 78 |
| 5497 | Efficient and Accurate Double-Hybrid-Meta-GGA Density Functionals Evaluation with the Extended GMTKN30 Database for General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 291-309. | 2.3 | 1,035 |
| 5498 | Discovering the chemical reactivity of the molecular oxonitride $[Ti(\hat{1}5-C_5Me_5)(\hat{1}4-O)]_3(\hat{1}43-N)$. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 4011-4017. | 0.8 | 9 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5499 | Arylation of styrene derivatives using aryliron complexes [CpFe(CO)2Ar] revealed by density functional theory calculations: Fe(II)-assisted group exchange through Fe-C bond cleavage and Fe-X bond formation. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 3852-3860. | 0.8 | 1 |
| 5500 | Tungsten(VI) N-Heterocyclic Carbene Complexes: Synthetic, Structural, and Computational Study. <i>Organometallics</i> , 2011, 30, 6262-6269. | 1.1 | 17 |
| 5501 | Understanding microsolvation of Li+: structural and energetical analyses. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 15264. | 1.3 | 38 |
| 5502 | Computational Evidence for the Role of Arabidopsis thaliana UVR8 as UV-B Photoreceptor and Identification of Its Chromophore Amino Acids. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 1287-1295. | 2.5 | 34 |
| 5503 | Sterically Governed Selectivity in Palladium-Assisted Allylic Alkylation. <i>Organometallics</i> , 2011, 30, 230-238. | 1.1 | 15 |
| 5504 | Linearity condition for orbital energies in density functional theory: Construction of orbital-specific hybrid functional. <i>Journal of Chemical Physics</i> , 2011, 134, 124113. | 1.2 | 34 |
| 5505 | How reliable are DFT transition structures? Comparison of GGA, hybrid-meta-GGA and meta-GGA functionals. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 689-700. | 1.5 | 212 |
| 5506 | Synthesis and structural characterization of group 6 transition metal complexes with terminal fluoromethylidyne (CF) ligands; a DFT/NBO/NRT comparison of bonding characteristics of terminal NO, CF and CH ligands. <i>Dalton Transactions</i> , 2011, 40, 47-55. | 1.6 | 19 |
| 5507 | The gauge including magnetically induced current method. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20500. | 1.3 | 326 |
| 5508 | Quantum Dots: Theory. , 2011, , 189-217. | | 2 |
| 5509 | Ring-Enlargement Reactions of Donor-Acceptor-Substituted Cyclopropanes: Which Combinations are Most Efficient?. <i>Organic Letters</i> , 2011, 13, 1848-1851. | 2.4 | 95 |
| 5510 | The Laplacian of Electron Density versus NICS-Scan: Measuring Magnetic Aromaticity among Molecules with Different Atom Types. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12708-12714. | 1.1 | 31 |
| 5511 | Analysis of the Effects of N-Substituents on Some Aspects of the Aromaticity of Imidazoles and Pyrazoles. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8571-8577. | 1.1 | 46 |
| 5512 | Substituents dependent capability of bis(ruthenium-dioxolene-terpyridine) complexes toward water oxidation. <i>Dalton Transactions</i> , 2011, 40, 2225-2233. | 1.6 | 36 |
| 5513 | X-ray Absorption Spectroscopic and Computational Investigation of a Possible S-S Interaction in the [Cu ₃ S ₂] ³⁺ Core. <i>Journal of the American Chemical Society</i> , 2011, 133, 17180-17191. | 6.6 | 29 |
| 5514 | Experimental and computational exploration of the dynamic behavior of (PNP)BF ₂ , a boron compound supported by an amido/bis(phosphine) pincer ligand. <i>Dalton Transactions</i> , 2011, 40, 11562. | 1.6 | 5 |
| 5515 | Cation Environment of BaCeO ₃ -Based Protonic Conductors II: New Computational Models. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1676-1685. | 1.1 | 4 |
| 5516 | Spin-adapted open-shell time-dependent density functional theory. III. An even better and simpler formulation. <i>Journal of Chemical Physics</i> , 2011, 135, 194106. | 1.2 | 57 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5517 | Comprehensive Benchmarking of a Density-Dependent Dispersion Correction. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3567-3577. | 2.3 | 400 |
| 5518 | Synthesis, Theoretical Study, and Antimicrobial Activity of Novel Polysubstituted Thiazoles. <i>Heterocycles</i> , 2011, 83, 1029. | 0.4 | 1 |
| 5519 | Structure and NMR Spectra of Some [2.2]Paracyclophanes. The Dilemma of [2.2]Paracyclophane Symmetry. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10638-10649. | 1.1 | 30 |
| 5520 | An unsymmetrical behavior of reactant units in the Kolbe-Schmitt reaction. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 891-900. | 0.5 | 2 |
| 5521 | Ring-Slippage and Multielectron Redox Properties of Fe/Ru/Os-Bis(arene) Complexes: Does Hapticity Change Really Cause Potential Inversion?. <i>Journal of the American Chemical Society</i> , 2011, 133, 18234-18242. | 6.6 | 15 |
| 5522 | Physico-Chemical Features of Aluminum Hydroxides As Modeled with the Hybrid B3LYP Functional and Localized Basis Functions. <i>Journal of Physical Chemistry C</i> , 2011, 115, 13107-13134. | 1.5 | 50 |
| 5523 | Interaction of Metal Ions with Biomolecular Ligands: How Accurate Are Calculated Free Energies Associated with Metal Ion Complexation?. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11394-11402. | 1.1 | 40 |
| 5524 | Self-assembly of metal-organic frameworks: From packing helical channels to 2-fold interpenetration helical layers. <i>CrystEngComm</i> , 2011, 13, 6373. | 1.3 | 4 |
| 5525 | Mechanism of intramolecular catalysis in the hydrolysis of alkyl monoesters of 1,8-naphthalic acid. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 6163. | 1.5 | 8 |
| 5526 | The effect of leaving group on mechanistic preference in phosphate monoester hydrolysis. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 5394. | 1.5 | 12 |
| 5527 | Experimental and Theoretical Study of Novel Luminescent Di-, Tri-, and Tetranuclear Copper Triazole Complexes. <i>Organometallics</i> , 2011, 30, 3275-3283. | 1.1 | 70 |
| 5528 | Molecular and computational structure characterizations of (E)-2-ethoxy-6-[(4-fluorophenylimino)methyl]phenol. <i>Journal of the Iranian Chemical Society</i> , 2011, 8, 674-686. | 1.2 | 2 |
| 5529 | Two-dimensional lattice oligomers of diboraspriopentadiene: a quantum chemical study. <i>Russian Chemical Bulletin</i> , 2011, 60, 2188-2195. | 0.4 | 2 |
| 5530 | Free-radical reactions of the tris-dioximate clathrochelates: synthesis and X-ray structure of the first cyclohexyl-substituted monoribbed-functionalized macrobicyclic iron(II) complex. <i>Russian Chemical Bulletin</i> , 2011, 60, 2504-2509. | 0.4 | 11 |
| 5531 | Thermodynamic and Kinetic Studies on Novel Dinuclear Platinum(II) Complexes Containing Bidentate N-donor ligands. <i>Inorganic Chemistry</i> , 2011, 50, 8984-8996. | 1.9 | 41 |
| 5532 | A Theoretical Investigation of the Plausibility of Reactions between Ammonia and Carbonyl Species (Formaldehyde, Acetaldehyde, and Acetone) in Interstellar Ice Analogs at Ultracold Temperatures. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5166-5183. | 1.1 | 30 |
| 5533 | Characterization of hydrogen dissociation over aluminium-doped zinc oxide using an efficient massively parallel framework for QM/MM calculations. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2011, 467, 1900-1924. | 1.0 | 21 |
| 5534 | Theoretical Prediction on the Thermal Stability of Cyclic Ozone and Strong Oxygen Tunneling. <i>Journal of the American Chemical Society</i> , 2011, 133, 16045-16053. | 6.6 | 35 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5535 | Exchange coupling in polynuclear nickel(II) complexes with pivalate and hexafluoroacetylacetonate ligands: a quantum chemical analysis. Russian Chemical Bulletin, 2011, 60, 2443-2450. | 0.4 | 0 |
| 5536 | Pressure Effects on the Quasi-1-D Molecular Ferromagnet 2-(4,5,6,7-Tetrafluorobenzimidazol-2-yl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazole-3-oxide-1-oxyl. Crystal Growth and Design, 2011, 11, 4261-4266. | 1.4 | 10 |
| 5537 | DFTB3: Extension of the Self-Consistent-Charge Density-Functional Tight-Binding Method (SCC-DFTB). Journal of Chemical Theory and Computation, 2011, 7, 931-948. | 2.3 | 828 |
| 5538 | 3,5-Diformylboron Dipyrromethenes as Fluorescent pH Sensors. Inorganic Chemistry, 2011, 50, 4392-4400. | 1.9 | 88 |
| 5539 | Performance of the van der Waals Density Functional VV10 and (hybrid)GGA Variants for Thermochemistry and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2011, 7, 3866-3871. | 2.3 | 213 |
| 5540 | Siloxane surfactant induced self-assembly of gold nanoparticles and their application to SERS. CrystEngComm, 2011, 13, 6179. | 1.3 | 52 |
| 5541 | Calorimetric and Computational Study of the Thermochemistry of Phenoxyphenols. Journal of Organic Chemistry, 2011, 76, 3754-3764. | 1.7 | 13 |
| 5542 | Electrochemical, EPR and computational results on [Fe2Cp2(CO)2]-based complexes with a bridging hydrocarbyl ligand. Journal of Organometallic Chemistry, 2011, 696, 3551-3556. | 0.8 | 10 |
| 5543 | ON ESTIMATING INTERSTELLAR POLYCYCLIC AROMATIC HYDROCARBON ABUNDANCES WITH CALCULATED OSCILLATOR STRENGTHS. Astrophysical Journal, 2011, 728, 62. | 1.6 | 5 |
| 5544 | Mechanical and Electronic Properties of Graphene Nanostructures. , 2011, , . | | 3 |
| 5545 | A Density Functional Theory Study of Chemical Functionalization of Carbon Nanotubes; Toward Site Selective Functionalization. , 0, , . | | 0 |
| 5546 | Predicting the UV-vis spectra of oxazine dyes. Beilstein Journal of Organic Chemistry, 2011, 7, 432-441. | 1.3 | 51 |
| 5547 | Chiral gold(I) vs chiral silver complexes as catalysts for the enantioselective synthesis of the second generation GSK-hepatitis C virus inhibitor. Beilstein Journal of Organic Chemistry, 2011, 7, 988-996. | 1.3 | 29 |
| 5548 | Mechanistic Study of ROS-photogeneration by Pterin. Pteridines, 2011, 22, 73-76. | 0.5 | 5 |
| 5549 | Toward an integrated route to the vernonia allenes and related sesquiterpenoids. Beilstein Journal of Organic Chemistry, 2011, 7, 937-943. | 1.3 | 16 |
| 5551 | Two-Photon Polarization Dependent Spectroscopy in Chirality: A Novel Experimental-Theoretical Approach to Study Optically Active Systems. Molecules, 2011, 16, 3315-3337. | 1.7 | 23 |
| 5552 | Catalytic Mechanism Investigation of Lysine-Specific Demethylase 1 (LSD1): A Computational Study. PLoS ONE, 2011, 6, e25444. | 1.1 | 42 |
| 5553 | Experimental and Modelling Studies of the Oxidation of Surrogate Bio-Aviation Fuels. , 2011, , . | | 0 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5554 | A COMPARATIVE STUDY OF META/PARA SUBSTITUTION EFFECTS ON THE HYDROGEN-BONDED COMPLEX OF ANILINE-H ₂ O: OBSERVATIONS FROM COMPUTATION. <i>Journal of Theoretical and Computational Chemistry</i> , 2011, 10, 567-579. | 1.8 | 2 |
| 5555 | Extraction Ability and Selectivity for Lithium Ion of Macrocyclic Trinuclear (Alkylbenzene)ruthenium(II) Complexes Bridged by 2,3-Pyridinediolato Ligands. <i>Bulletin of the Chemical Society of Japan</i> , 2011, 84, 259-265. | 2.0 | 4 |
| 5558 | Comparison of Inhibitory Activities of Stereo-Isomers of Cyclic Phosphatidic Acid (cPA) on Autotaxin. <i>Cytologia</i> , 2011, 76, 73-80. | 0.2 | 4 |
| 5559 | The intriguing modeling of <i>cis</i> vs <i>trans</i> selectivity in ruthenium-catalyzed olefin metathesis. <i>Beilstein Journal of Organic Chemistry</i> , 2011, 7, 40-45. | 1.3 | 31 |
| 5561 | Brueckner doubles coupled cluster method with the polarizable continuum model of solvation. <i>Journal of Chemical Physics</i> , 2011, 134, 244113. | 1.2 | 19 |
| 5562 | PROTONATED POLYCYCLIC AROMATIC HYDROCARBONS REVISITED. <i>Astrophysical Journal</i> , 2011, 727, 128. | 1.6 | 15 |
| 5563 | Dissociative double photoionization of singly deuterated benzene molecules in the 26-33 eV energy range. <i>Journal of Chemical Physics</i> , 2011, 135, 144304. | 1.2 | 34 |
| 5564 | Hydrogen and oxygen adsorption on a nanosilicate - a quantum chemical study. <i>Monthly Notices of the Royal Astronomical Society</i> , 2011, 414, 1285-1291. | 1.6 | 27 |
| 5565 | Terahertz, infrared and Raman vibrational assignments of [FeFe]-hydrogenase model compounds. <i>Vibrational Spectroscopy</i> , 2011, 56, 219-227. | 1.2 | 11 |
| 5566 | A theoretical study of keto-enol isomerism and internal rotation in the H ₂ Salen molecule, N,N'-ethylene-bis(salicylideneimine) Schiff base. <i>Journal of Structural Chemistry</i> , 2011, 52, 16-26. | 0.3 | 10 |
| 5567 | Structure and DFT calculations of <i>Chemistry</i> , 2011, 52, 596-601. | 0.3 | 6 |
| 5568 | Twisted molecular geometry and localized electronic structure of the triplet excited gem-diphenyltrimethylenemethane biradical: substituent effects on thermoluminescence and related theoretical calculations. <i>Tetrahedron</i> , 2011, 67, 7431-7439. | 1.0 | 12 |
| 5569 | Synthesis and characterization of permethylated 1,3,5-tri- and 1,3,5,7-tetracarbonyl compounds. <i>Tetrahedron</i> , 2011, 67, 8780-8789. | 1.0 | 6 |
| 5570 | Exploring the mechanism for the amine-catalyzed isomerization of dimethyl maleate. A computational study. <i>Tetrahedron Letters</i> , 2011, 52, 6288-6294. | 0.7 | 10 |
| 5571 | Spectroscopic and theoretical studies of some N,N-diethyl-2-[(4-substituted)phenylsulfonyl]acetamides. <i>Journal of Molecular Structure</i> , 2011, 1002, 97-106. | 1.8 | 8 |
| 5572 | Synthesis, crystal structures and DFT studies of 1-[2-(5-methyl-2-benzoxazolinone-3-yl)acetyl]-3-phenyl-5-(3,4-dimethoxyphenyl)-4,5-dihydro-1H-pyrazole and 1-[2-(5-chloro-2-benzoxazolinone-3-yl)acetyl]-3-phenyl-5-(4-methoxyphenyl)-4,5-dihydro-1H-pyrazole. <i>Journal of Molecular Structure</i> , 2011, 1006, 147-158. | 1.8 | 15 |
| 5573 | Experimental and computational study on the molecular energetics of benzyloxyphenol isomers. <i>Journal of Chemical Thermodynamics</i> , 2011, 43, 1857-1864. | 1.0 | 7 |
| 5574 | Probing the compound (E)-5-(diethylamino)-2-[(4-methylphenylimino)methyl]phenol mainly from the point of tautomerism in solvent media and the solid state by experimental and computational methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 72-78. | 2.0 | 30 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5575 | A characterization study on 2,6-dimethyl-4-nitropyridine N-oxide by density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 104-110. | 2.0 | 10 |
| 5576 | Vibrational spectroscopy investigation and HOMO, LUMO analysis using DFT (B3LYP) on the structure of 1,3-dichloro 5-nitrobenzene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 242-50. | 2.0 | 4 |
| 5577 | Synthesis, X-ray crystal structure and fluorescent spectra of novel pyrazolo[1,5-a]pyrazin-4(5H)-one derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 372-379. | 2.0 | 5 |
| 5578 | Theoretical investigation of the molecular structures and excitation spectra of triphenylamine and its derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 653-660. | 2.0 | 7 |
| 5579 | Experimental (¹³ C NMR, ¹ H NMR, FT-IR, single-crystal X-ray diffraction) and DFT studies on 3,4-bis(isopropylamino)cyclobut-3-ene-1,2-dione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 83, 472-477. | 2.0 | 4 |
| 5580 | Investigation into the shape selectivity of zeolite catalysts for biomass conversion. <i>Journal of Catalysis</i> , 2011, 279, 257-268. | 3.1 | 963 |
| 5581 | Methyltrioxorhenium-catalyzed oxidation of pseudocumene for vitamin E synthesis: A study of solvent and ligand effects. <i>Journal of Catalysis</i> , 2011, 283, 55-67. | 3.1 | 32 |
| 5582 | Kinetic parameters of abstraction reactions of OH radical with ethylene, fluoroethylene, cis- and trans-1,2-difluoroethylene and 1,1-difluoroethylene, in the temperature range of 200–400K: Gaussian-3/B3LYP theory. <i>Chemical Physics Letters</i> , 2011, 511, 440-446. | 1.2 | 11 |
| 5583 | On the electronic structure of mono-rhenium oxide clusters: and ReO _n (n=3,4). <i>Chemical Physics Letters</i> , 2011, 512, 49-53. | 1.2 | 15 |
| 5584 | The Fukui potential is a measure of the chemical hardness. <i>Chemical Physics Letters</i> , 2011, 513, 127-129. | 1.2 | 34 |
| 5585 | Linearity condition for orbital energies in density functional theory (II): Application to global hybrid functionals. <i>Chemical Physics Letters</i> , 2011, 513, 130-135. | 1.2 | 28 |
| 5586 | Theoretical calculations of the excited state potential energy surfaces of nitric oxide. <i>Chemical Physics Letters</i> , 2011, 513, 179-183. | 1.2 | 23 |
| 5587 | An electrochromic diquat-quaterthiophene alternating copolymer: A polythiophene with a viologen-like moiety in the main chain. <i>Electrochimica Acta</i> , 2011, 56, 8108-8114. | 2.6 | 17 |
| 5588 | Probing valence and spin situations in selective ruthenium–iminoquinonoid frameworks. An experimental and DFT analysis. <i>Inorganica Chimica Acta</i> , 2011, 374, 216-225. | 1.2 | 11 |
| 5589 | Spectro-electrochemical and DFT studies of a planar Cu(II)–phenolate complex active in the aerobic oxidation of primary alcohols. <i>Inorganica Chimica Acta</i> , 2011, 374, 406-414. | 1.2 | 19 |
| 5590 | Preparation, structural, spectroscopic, thermal and DFT characterization of cadmium(II) complexes with quinaldic acid. <i>Inorganica Chimica Acta</i> , 2011, 378, 154-162. | 1.2 | 14 |
| 5591 | Design, synthesis and biological evaluation of mannosyl triazoles as FimH antagonists. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 6454-6473. | 1.4 | 77 |
| 5592 | Effect of different C3-aryl substituents on the antioxidant activity of 4-hydroxycoumarin derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 6233-6238. | 1.4 | 39 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 5593 | The role of correlations in the high-pressure phase of FeSe. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 205601. | 0.7 | 5 |
| 5594 | A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6670. | 1.3 | 1,627 |
| 5595 | Assessment of the Performance of DFT and DFT-D Methods for Describing Distance Dependence of Hydrogen-Bonded Interactions. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 88-96. | 2.3 | 388 |
| 5596 | Interactions of polysulfanes with components of red blood cells. <i>MedChemComm</i> , 2011, 2, 196. | 3.5 | 26 |
| 5597 | Optical Rotation Calculated with Time-Dependent Density Functional Theory: The OR45 Benchmark. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10930-10949. | 1.1 | 110 |
| 5598 | Reliability of Hybrid Functionals in Predicting Band Gaps. <i>Physical Review Letters</i> , 2011, 107, 216806. | 2.9 | 150 |
| 5599 | Influence of Triplet Instabilities in TDDFT. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3578-3585. | 2.3 | 285 |
| 5600 | Dispersion, static correlation, and delocalisation errors in density functional theory: An electrostatic theorem perspective. <i>Journal of Chemical Physics</i> , 2011, 135, 164110. | 1.2 | 10 |
| 5601 | Layered hydroxide hybrid nanostructures: a route to multifunctionality. <i>Chemical Society Reviews</i> , 2011, 40, 1031. | 18.7 | 137 |
| 5602 | Elemental Reactions in Copolymerization of $\hat{1}\pm$ -Olefins by Bis(cyclopentadienyl) Zirconocene and Hafnocene: Effects of the Metal as a Function of the Monomer and the Chain End. <i>Organometallics</i> , 2011, 30, 1350-1358. | 1.1 | 26 |
| 5603 | Fundamental and excitation gaps in molecules of relevance for organic photovoltaics from an optimally tuned range-separated hybrid functional. <i>Physical Review B</i> , 2011, 84, . | 1.1 | 281 |
| 5604 | Long-range corrected hybrid functionals for $\hat{1}\epsilon$ -conjugated systems: Dependence of the range-separation parameter on conjugation length. <i>Journal of Chemical Physics</i> , 2011, 135, 204107. | 1.2 | 234 |
| 5605 | Density-functional approaches to noncovalent interactions: A comparison of dispersion corrections (DFT-D), exchange-hole dipole moment (XDM) theory, and specialized functionals. <i>Journal of Chemical Physics</i> , 2011, 134, 084107. | 1.2 | 607 |
| 5606 | Interpretation of substituent effects on ^{13}C and ^{15}N NMR chemical shifts in 6-substituted purines. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 15854. | 1.3 | 31 |
| 5607 | Synthesis, Reactivity, and Properties of N-Fused Porphyrin Manganese(I) Tricarbonyl Complexes. <i>Inorganic Chemistry</i> , 2011, 50, 6029-6043. | 1.9 | 42 |
| 5608 | Pharmaceutical Co-crystals with Isonicotinamide $\hat{1}\epsilon$ "Vitamin B3, Clofibric Acid, and Diclofenac $\hat{1}\epsilon$ "and Two Isonicotinamide Hydrates. <i>Crystal Growth and Design</i> , 2011, 11, 75-87. | 1.4 | 115 |
| 5609 | Carbocations or Cyclopropyl Gold Carbenes in Cyclizations of Enynes. <i>Chemistry - an Asian Journal</i> , 2011, 6, 482-486. | 1.7 | 31 |
| 5610 | Selectivities in Chiral Lewis Acid Catalyzed Diels $\hat{1}\epsilon$ "Alder Reactions of Acetylenic Ketones: Explanation for Differences of Selectivities between Acyclic and Cyclic Dienes. <i>Chemistry - an Asian Journal</i> , 2011, 6, 380-384. | 1.7 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5611 | Intramolecular Aromatic Carbenoid Insertion of Biaryldiazoacetates for the Regioselective Synthesis of Fluorenes. <i>Chemistry - an Asian Journal</i> , 2011, 6, 2040-2047. | 1.7 | 34 |
| 5612 | Mechanism of Side Reactions in Alkane C-H Bond Functionalization by Diazo Compounds Catalyzed by Ag and Cu Homoscorpionate Complexes—A DFT Study. <i>ChemCatChem</i> , 2011, 3, 1646-1652. | 1.8 | 47 |
| 5613 | Assessing computationally efficient isomerization dynamics: $\hat{\rho}^n$ SCF density-functional theory study of azobenzene molecular switching. <i>Journal of Chemical Physics</i> , 2011, 135, 224303. | 1.2 | 53 |
| 5614 | Disentanglement of triplet and singlet states of azobenzene: direct EELS detection and QMC modeling. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20939. | 1.3 | 20 |
| 5615 | Structures and Stabilities of Fe ^{2+/3+} Complexes Relevant to Alzheimer's Disease: An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12523-12530. | 1.1 | 27 |
| 5616 | Role of NO ⁺ Intermediates in NO Reduction with Propene over NiZSM-5 Zeolite Revealed by EPR and IR Spectroscopic Investigations and DFT Modeling. <i>Journal of Physical Chemistry C</i> , 2011, 115, 13008-13015. | 1.5 | 24 |
| 5617 | Direct probing of ion pair formation using a symmetric triangulenium dye. <i>Photochemical and Photobiological Sciences</i> , 2011, 10, 1963-1973. | 1.6 | 26 |
| 5618 | Stability and properties of oligomeric organoboron structures with six-coordinate carbon atoms at centers of hydrocarbon frameworks. <i>Russian Chemical Bulletin</i> , 2011, 60, 1525-1530. | 0.4 | 0 |
| 5619 | Calculations of ionization energies and electron affinities for atoms and molecules: A comparative study with different methods. <i>Frontiers of Chemistry in China: Selected Publications From Chinese Universities</i> , 2011, 6, 269-279. | 0.4 | 22 |
| 5620 | Transition metal complexes with 2-(N-tosylamino)benzaldehyde 1-phthalazinylohydrazone. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2011, 37, 483-491. | 0.3 | 20 |
| 5621 | Quantum-chemical study of reaction mechanism between tris(2-hydroxyethyl)ammonium fluoride and tetraethoxysilane. <i>Russian Journal of General Chemistry</i> , 2011, 81, 1792-1797. | 0.3 | 1 |
| 5622 | Chemistry of naphthazarin derivatives: XV. Bromination of naphthazarin and its derivatives. <i>Russian Journal of Organic Chemistry</i> , 2011, 47, 504-509. | 0.3 | 1 |
| 5623 | Tautomeric and conformational equilibria of $\hat{\rho}^3$ -lactones derived from (3,5-dibromo-1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)acetic acid. <i>Russian Journal of Organic Chemistry</i> , 2011, 47, 1487-1491. | 0.3 | 1 |
| 5624 | IR Vibrational spectra of H-bonded complexes of adenine, 2-aminopurine and 2-aminopurine+ with cytosine and thymine: Quantum-chemical study. <i>Optics and Spectroscopy (English Translation of Tj ETQq1 1 0.784314 rgBT4/5 Overload)</i> | 0.3 | 1 |
| 5625 | New approach to determine absolute partial pressures of ions in saturated vapors of inorganic materials. <i>Russian Journal of Inorganic Chemistry</i> , 2011, 56, 1312-1317. | 0.3 | 2 |
| 5626 | Dimer-covering resonating-valence-bond treatment of single-walled zigzag carbon nanotubes. <i>European Physical Journal B</i> , 2011, 80, 469-475. | 0.6 | 0 |
| 5627 | Geometries and electronic structures of Ga ₂ Se ₃ , Ga ₃ Se ₂ and their anions. Theoretical insights. <i>European Physical Journal D</i> , 2011, 63, 351-358. | 0.6 | 3 |
| 5628 | How Well Can Modern Density Functionals Predict Internuclear Distances at Transition States?. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1667-1676. | 2.3 | 156 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 5629 | Characterization of Dimeric Chiral Lithium Amide Structures Derived from N-isopropyl-O-triisopropylsilyl Valinol. <i>Journal of the American Chemical Society</i> , 2011, 133, 6596-6602. | 6.6 | 29 |
| 5630 | Decarboxylative coupling reactions: a modern strategy for C-C bond formation. <i>Chemical Society Reviews</i> , 2011, 40, 5030. | 18.7 | 1,241 |
| 5631 | Redox Properties of Tanaka's Water Oxidation Catalyst: Redox Noninnocent Ligands Dominate the Electronic Structure and Reactivity. <i>Inorganic Chemistry</i> , 2011, 50, 5946-5957. | 1.9 | 35 |
| 5632 | On the Structural and Electronic Properties of $[Zn_2(4,4\text{-bipyridine})(mes)_4]^{2+}$, a Homologous Series of Bimetallic Complexes Bridged by Neutral, Anionic, and Dianionic 4,4'-Bipyridine. <i>Inorganic Chemistry</i> , 2011, 50, 5006-5014. | 1.9 | 25 |
| 5633 | New chemistry of 1,2-closo-P2B10H10 and 1,2-closo-As2B10H10; in silico and gas electron diffraction structures, and new metalladiphospha- and metalladiarsaboranes. <i>Dalton Transactions</i> , 2011, 40, 7181. | 1.6 | 21 |
| 5634 | Electrochemistry of graphene: not such a beneficial electrode material?. <i>RSC Advances</i> , 2011, 1, 978. | 1.7 | 217 |
| 5635 | Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3944-3951. | 2.3 | 265 |
| 5636 | Density Functional Theory for Reaction Energies: Test of Meta and Hybrid Meta Functionals, Range-Separated Functionals, and Other High-Performance Functionals. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 669-676. | 2.3 | 190 |
| 5637 | Density Functional Calculations. , 2011, , 445-519. | | 3 |
| 5638 | Excited-state calculations with TD-DFT: from benchmarks to simulations in complex environments. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16987. | 1.3 | 301 |
| 5639 | Improving the Accuracy of Hybrid Meta-GGA Density Functionals by Range Separation. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2810-2817. | 2.1 | 864 |
| 5640 | Density functional theory with London dispersion corrections. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 211-228. | 6.2 | 2,030 |
| 5641 | DNA insertion in and wrapping around carbon nanotubes. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 902-919. | 6.2 | 6 |
| 5642 | Modeling of structures and calculation of IR vibrational spectra of N,N-dimethylformamide dimers by density functional theory. <i>Journal of Applied Spectroscopy</i> , 2011, 78, 326-336. | 0.3 | 39 |
| 5643 | Manifestation of enol-enol tautomerism in IR spectra of 2-acetylcyclopentanone-d1. <i>Journal of Applied Spectroscopy</i> , 2011, 78, 489-500. | 0.3 | 3 |
| 5644 | Naphthyridine amide-urea conjugate: a case toward selective fluorometric sensing of N-acetyl proline carboxylate. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2011, 71, 243-248. | 1.6 | 3 |
| 5645 | Electronic Properties and Chemical Bonding of O-Rich Clusters $M_2O_7^{2-}$ (M, $\text{M}=\text{V}, \text{Nb}, \text{Ta}$). <i>Journal of Cluster Science</i> , 2011, 22, 397-404. | 1.7 | 1 |
| 5646 | Influence of Prototropic Reactions on the Absorption and Fluorescence Spectra of Methyl p-dimethylaminobenzoate and Its Two Ortho Derivatives. <i>Journal of Fluorescence</i> , 2011, 21, 1749-1762. | 1.3 | 12 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5647 | Polymerization of p-nitrobenzyl acrylate under microwave irradiation and their optical properties. <i>Journal of Polymer Research</i> , 2011, 18, 1293-1299. | 1.2 | 1 |
| 5648 | Dibromotyrosine derivatives from the ethanol extract of the marine sponge <i>Aplysina</i> sp.: structures, transformations, and origin. <i>Russian Chemical Bulletin</i> , 2011, 60, 570-580. | 0.4 | 8 |
| 5649 | 7-Ethyl-2,3,5,6,8-pentahydroxy-1,4-naphthoquinone (echinochrome A): a DFT study of the mechanism of the antioxidant action. 4. Migration of protons and the Na ⁺ cation in echinochrome a monosodium salts. <i>Russian Chemical Bulletin</i> , 2011, 60, 639-646. | 0.4 | 1 |
| 5650 | Ab initio and DFT conformational study on nitrosamine (H ₂ N-N=O) and N-Nitrosodimethylamine [(CH ₃) ₂ N-N=O]. <i>Structural Chemistry</i> , 2011, 22, 497-507. | 1.0 | 10 |
| 5651 | A DFT quantum mechanical study of 3-hydroxy-4-pyrone and 3-hydroxy-4-pyridinone based oxidovanadium(IV) complexes. <i>Structural Chemistry</i> , 2011, 22, 697-706. | 1.0 | 7 |
| 5652 | Oxygen cleavage with manganese and iron in ribonucleotide reductase from <i>Chlamydia trachomatis</i> . <i>Journal of Biological Inorganic Chemistry</i> , 2011, 16, 553-565. | 1.1 | 26 |
| 5653 | The mechanism of formate oxidation by metal-dependent formate dehydrogenases. <i>Journal of Biological Inorganic Chemistry</i> , 2011, 16, 1255-1268. | 1.1 | 75 |
| 5654 | First principles calculations of the electronic and chemical properties of graphene, graphane, and graphene oxide. <i>Journal of Molecular Modeling</i> , 2011, 17, 1133-1139. | 0.8 | 153 |
| 5655 | Mechanistic investigation of the base-promoted cycloselenoetherification of pent-4-en-1-ol. <i>Journal of Molecular Modeling</i> , 2011, 17, 1251-1257. | 0.8 | 15 |
| 5656 | A new scheme to calculate isotope effects. <i>Journal of Molecular Modeling</i> , 2011, 17, 2175-2182. | 0.8 | 3 |
| 5657 | Electronic structure study using density functional theory in organic dendrimers. <i>Journal of Molecular Modeling</i> , 2011, 17, 1963-1972. | 0.8 | 8 |
| 5658 | Computational design and structure-property relationship studies on heptazines. <i>Journal of Molecular Modeling</i> , 2011, 17, 2927-2937. | 0.8 | 13 |
| 5659 | A theoretical thermodynamic investigation of cascade reactions in dinuclear octa-azacryptates involving carbon dioxide. <i>Journal of Molecular Modeling</i> , 2011, 17, 3151-3162. | 0.8 | 6 |
| 5660 | Adsorption and spin state properties of Cr, Ni, Mo, and Pt deposited on Li ⁺ and Na ⁺ monovalent cation impurities of MgO (001) surface: DFT calculations. <i>Journal of Molecular Modeling</i> , 2011, 17, 3299-3308. | 0.8 | 7 |
| 5661 | Computational analysis of tris(1,2-ethanediamine) cobalt(III) complex ion: calculation of the ⁵⁹ Co shielding tensor using LF-DFT. <i>Monatshefte für Chemie</i> , 2011, 142, 593-597. | 0.9 | 11 |
| 5662 | Magnetic Properties of Monomer and Dimer Tetrahedral VO _x Entities Dispersed on Amorphous Silica-based Materials: Prediction of EPR Parameters from Relativistic DFT Calculations and Broken Symmetry Approach to Exchange Couplings. <i>Applied Magnetic Resonance</i> , 2011, 40, 471-479. | 0.6 | 6 |
| 5663 | Nuclear magnetic resonance parameters in water dimer. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 313-324. | 0.5 | 6 |
| 5664 | Aromaticity and electronic delocalization in all-metal clusters with single, double, and triple aromatic character. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 419-431. | 0.5 | 57 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5665 | The importance of conformational search: a test case on the catalytic cycle of the Suzuki–Miyaura cross-coupling. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 639-646. | 0.5 | 67 |
| 5666 | Molecular structure of cyanidin metal complexes: Al(III) versus Mg(II). <i>Theoretical Chemistry Accounts</i> , 2011, 128, 485-495. | 0.5 | 18 |
| 5667 | Performance of density functional theory on homogeneous gold catalysis. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 647-661. | 0.5 | 81 |
| 5668 | Minimally augmented Karlsruhe basis sets. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 295-305. | 0.5 | 638 |
| 5669 | Electric field effects on nuclear spin–spin coupling tensors and chiral discrimination via NMR spectroscopy. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 359-366. | 0.5 | 18 |
| 5670 | A density functional theory study of the manganese-phthalocyanine. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 497-503. | 0.5 | 30 |
| 5671 | Theoretical study of the gas-phase Fe ⁺ -mediated oxidation of ethane by N ₂ O. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 349-358. | 0.5 | 8 |
| 5672 | Mössbauer spectroscopy for heavy elements: a relativistic benchmark study of mercury. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 631-650. | 0.5 | 61 |
| 5673 | How accurate are electronic structure methods for actinoid chemistry?. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 657-666. | 0.5 | 65 |
| 5674 | Relativistic four-component calculations of Buckingham birefringence using London atomic orbitals. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 685-699. | 0.5 | 4 |
| 5675 | The geometric, energetic, and electronic properties of charged phosphorus-doped silicon clusters, Ψ_n^+/Ψ_n^- ($n=1-8$). <i>Theoretical Chemistry Accounts</i> , 2011, 130, 1009-1022. | 0.5 | 7 |
| 5676 | Finite-field evaluation of static (hyper)polarizabilities based on the linear-scaling divide-and-conquer method. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 701-709. | 0.5 | 14 |
| 5677 | Assessment of theoretical procedures for hydrogen-atom abstraction by chlorine, and related reactions. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 251-260. | 0.5 | 37 |
| 5678 | What is the best density functional to describe water clusters: evaluation of widely used density functionals with various basis sets for (H ₂ O) _n ($n=1-10$). <i>Theoretical Chemistry Accounts</i> , 2011, 130, 341-352. | 0.5 | 46 |
| 5679 | DFT studies of cation binding by β -cyclodextrin. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 939-953. | 0.5 | 33 |
| 5681 | A B3LYP investigation of the conformational and environmental sensitivity of carbon–deuterium frequencies of aryl-perdeuterated phenylalanine and tryptophan. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 883-889. | 0.5 | 4 |
| 5682 | A theoretical approach to molecular single-electron transistors. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 839-850. | 0.5 | 9 |
| 5683 | Intra-cluster proton transfer in anilide–(HF) _n ($n=1-4$): Can the size of HF cluster influence the N ₃ H ⁺ –H ₂ N ⁺ switching. <i>Journal of Fluorine Chemistry</i> , 2011, 132, 459-467. | 0.9 | 9 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5684 | Theoretical study of new acceptor and donor molecules based on polycyclic aromatic hydrocarbons. <i>Journal of Molecular Spectroscopy</i> , 2011, 265, 95-101. | 0.4 | 27 |
| 5685 | Synthesis and characterization of ethylenediaminium nitrophenolate. <i>Journal of Molecular Structure</i> , 2011, 989, 136-143. | 1.8 | 18 |
| 5686 | Structure of 3,4-dicarboxy-1-methylpyridinium inner salt studied by X-ray diffraction, DFT calculations, FTIR, Raman and NMR spectra. <i>Journal of Molecular Structure</i> , 2011, 994, 216-222. | 1.8 | 10 |
| 5687 | Structure and vibrational assignment of tautomerism of 4-hydroxyquinazoline in gaseous and aqueous phases. <i>Journal of Molecular Structure</i> , 2011, 1001, 16-22. | 1.8 | 8 |
| 5688 | FT-IR and computational study of (E)-N-carbamimidoyl-4-((2-formylbenzylidene)amino)benzene sulfonamide. <i>Journal of Molecular Structure</i> , 2011, 1001, 29-35. | 1.8 | 26 |
| 5689 | Probing the compound (E)-2-[(4-bromophenylimino)methyl]-6-ethoxyphenol mainly from the point of tautomerism in solvent media and the solid state by experimental and computational methods. <i>Journal of Molecular Structure</i> , 2011, 1000, 162-170. | 1.8 | 25 |
| 5690 | Potential energy surfaces and mechanisms for activation of ethane by gas-phase Pt ⁺ : A density functional study. <i>Chemical Physics Letters</i> , 2011, 501, 554-561. | 1.2 | 11 |
| 5691 | Applications and validations of the Minnesota density functionals. <i>Chemical Physics Letters</i> , 2011, 502, 1-13. | 1.2 | 662 |
| 5692 | The infrared spectrum of spessartine  overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www.elsevie.chemic"/> Functionalizable magnetic/luminous silicon/bismuth core/shell nanocrystalline particles. <i>Chemical Physics Letters</i> , 2011, 508, 252-257. | 1.2 | 19 |
| 5693 | Functionalizable magnetic/luminous silicon/bismuth core/shell nanocrystalline particles. <i>Chemical Physics Letters</i> , 2011, 508, 252-257. | 1.2 | 1 |
| 5694 | DFT, FT-Raman, FT-IR, solution and solid state NMR studies of 2,4-dimethoxyphenylboronic acid. <i>Comptes Rendus Chimie</i> , 2011, 14, 446-455. | 0.2 | 15 |
| 5695 | Effect of alkali on methylene blue (C.I. Basic Blue 9) and other thiazine dyes. <i>Dyes and Pigments</i> , 2011, 88, 149-155. | 2.0 | 97 |
| 5696 | Electronic structures and reactivity aspects of ruthenium nitrosyls. <i>Inorganica Chimica Acta</i> , 2011, 372, 250-258. | 1.2 | 15 |
| 5697 | Theoretical study of lanthanide mono cation-mediated C-F bond activation. <i>Chemical Physics</i> , 2011, 380, 48-53. | 0.9 | 11 |
| 5698 | Construction of orbital-specific hybrid functional by imposing the linearity condition for orbital energies in density functional theory. <i>Procedia Computer Science</i> , 2011, 4, 1151-1156. | 1.2 | 2 |
| 5699 | Vibrational spectroscopic studies of N,N-dimethylpropyleneurea-water system: Affected solvent spectra and factor analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 712-721. | 2.0 | 6 |
| 5700 | Characterization of pentacarbonyl(4-methylpyridine)chromium(0) complex using density functional theory (DFT) and Hartree-Fock (HF) computational methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 1715-1721. | 2.0 | 9 |
| 5701 | Determination of the absolute configuration of the enantiomers of dihydroquinolines, isolated by chiral chromatography, by non empirical analysis of circular dichroism spectra and X-ray analysis. <i>Tetrahedron: Asymmetry</i> , 2011, 22, 270-276. | 1.8 | 1 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5702 | Electron-Capture and -Transfer Dissociation of Peptides Tagged with Tunable Fixed-Charge Groups: Structures and Dissociation Energetics. <i>Journal of the American Society for Mass Spectrometry</i> , 2011, 22, 13-30. | 1.2 | 11 |
| 5703 | Dipole-Guided Electron Capture Causes Abnormal Dissociations of Phosphorylated Pentapeptides. <i>Journal of the American Society for Mass Spectrometry</i> , 2011, 22, 731-751. | 1.2 | 36 |
| 5704 | Density functional theory study of the mechanism of the acid-catalyzed decarboxylation of pyrrole-2-carboxylic acid and mesitoic acid. <i>Science China Chemistry</i> , 2011, 54, 762-768. | 4.2 | 8 |
| 5705 | [Be ₃ ($\frac{1}{4}$) ₃ O ₃](MeCN) ₆ {Be(MeCN) ₃ } ₃ (l) ₆ – ein Berylliumkomplex mit Cyclohexaborat-Kern und sein Hydrolyseprodukt [Be(H ₂ O) ₄](l) ₂ MeCN. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2011, 637, 67-74. | 0.6 | 16 |
| 5706 | Ligand Exchange Processes on Solvated Beryllium Cations V. Water Exchange on [Be(X)(H ₂ O) ₃] ⁺ (X: H ₂ O, F ⁻ , Cl ⁻ , Tl ⁺ , Cs ⁺ , Rb ⁺ , K ⁺ , NH ₄ ⁺). <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2011, 637, 515-522. | 0.6 | 11 |
| 5707 | Molecular Structure and Antimicrobial Activity of a Luminescent Dinuclear Silver(I) Complex of Phenylbis(2-pyridyl)phosphine. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2011, 637, 2260-2264. | 0.6 | 9 |
| 5708 | Molecular Structures of a 1,5-Diseleno-2,4-disila-3-oxa-cycloheptane Derivative and a Diselane. Behavior of the Mixture Containing 1,2-Dithio- and 1,2-Bis(lithioselena)-1,2-dicarba-closo-dodecaborane(12). <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2011, 637, 1895-1902. | 0.6 | 4 |
| 5709 | [Be(Chelate)Sol] ₂ ²⁺ (Chelate: Tl ⁺ , Cs ⁺ , Rb ⁺ , K ⁺ , NH ₄ ⁺). <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2011, 637, 515-522. | 0.6 | 4 |
| 5710 | Molecular origins of commercial laser dye functionality in azacoumarins and 2-quinolones: LD 425, LD 489 and LD 473. <i>Acta Crystallographica Section B: Structural Science</i> , 2011, 67, 560-568. | 1.8 | 6 |
| 5711 | SiO ₂ in density functional theory and beyond. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 1061-1066. | 0.7 | 15 |
| 5712 | Accurate treatment of solids with the HSE screened hybrid. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 767-774. | 0.7 | 258 |
| 5713 | Organocatalytic depolymerization of poly(ethylene terephthalate). <i>Journal of Polymer Science Part A</i> , 2011, 49, 1273-1281. | 2.5 | 172 |
| 5714 | Synthesis, characterization, and computational modeling of benzodithiophene donor-acceptor semiconducting polymers. <i>Journal of Polymer Science Part A</i> , 2011, 49, 4172-4179. | 2.5 | 11 |
| 5715 | Oxidation potential of thiophene oligomers: Theoretical and experimental approach. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2011, 49, 1723-1733. | 2.4 | 39 |
| 5716 | Cell response of <i>Escherichia coli</i> to cisplatin-induced stress. <i>Proteomics</i> , 2011, 11, 4174-4188. | 1.3 | 19 |
| 5717 | The stability and reactivity of activated acryloylcarbamates as reagents for the synthesis of <i>N</i> -substituted thymine and uracil – an NMR and DFT study. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 423-430. | 0.9 | 2 |
| 5718 | Fundamental properties of <i>N</i> -alkenylaziridines – implications for the design of new reactions and organocatalysts. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 445-449. | 0.9 | 1 |
| 5719 | Theoretical studies on aromaticity of selected hydroxypyrones. Part 3#. Chelatoaromaticity phenomenon in metalcomplexes of hydroxypyrones. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 499-506. | 0.9 | 16 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5720 | Studies of gas-phase reactions of cationic iron complexes of 2-pyrimidinyloxy-N-arylamines by electrospray ionization tandem mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2011, 25, 169-178. | 0.7 | 8 |
| 5721 | Density functional theory study of B _n C clusters. <i>Rapid Communications in Mass Spectrometry</i> , 2011, 25, 1315-1322. | 0.7 | 5 |
| 5722 | Dependence of collision-induced dissociation energy on molecular degrees of freedom as a means to assess relative binding affinity in multivalent complexes. <i>Rapid Communications in Mass Spectrometry</i> , 2011, 25, 2299-2306. | 0.7 | 3 |
| 5723 | DFT performance for the hole transfer parameters in DNA π stacks. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 191-201. | 1.0 | 23 |
| 5724 | Exchange and correlation in density functional theory and quantum chemistry. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 563-569. | 1.0 | 10 |
| 5725 | First principles investigation on the key factors of broad absorption spectra and electronic properties for oligothiophene and its derivatives for solar cells. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2089-2098. | 1.0 | 12 |
| 5726 | New nonsteroidal anti-inflammatory molecules with reduced photodegradation side effects and enhanced COX-2 selectivity. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1184-1195. | 1.0 | 6 |
| 5727 | Density functional theory study of the structure and energetics of negatively charged oligopyrroles. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2295-2305. | 1.0 | 56 |
| 5728 | Interaction of the Mn ²⁺ , Co ²⁺ , Ni ²⁺ , and Zn ²⁺ with prion protein HGGGW pentapeptide model. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1152-1162. | 1.0 | 8 |
| 5729 | CHARMM-based parameterization of neutral articaine. A widely used local anesthetic. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1339-1345. | 1.0 | 8 |
| 5730 | Advances in local hybrid exchange-correlation functionals: from thermochemistry to magnetic resonance parameters and hyperpolarizabilities. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2625-2638. | 1.0 | 42 |
| 5731 | A first principles investigation of the hydrogen bond interaction and the sensitive characters in <i>cis</i> -1,3,4,6-tetranitrooctahydroimidazo[4,5-d]imidazole. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 4457-4464. | 1.0 | 11 |
| 5732 | Protonation sites and dissociation mechanisms of <i>t</i> -butylcarbamates in tandem mass spectrometric assays for newborn screening. <i>Journal of Mass Spectrometry</i> , 2011, 46, 1089-1098. | 0.7 | 15 |
| 5733 | ¹ H, ¹³ C, ¹⁵ N NMR coordination shifts in Fe(II), Ru(II) and Os(II) cationic complexes with 2,2':6',2''-terpyridine. <i>Magnetic Resonance in Chemistry</i> , 2011, 49, 237-241. | 1.1 | 17 |
| 5734 | Isotopic effect on tautomeric behavior of 5-(2,6-disubstituted-aryloxy)-tetrazoles. <i>Magnetic Resonance in Chemistry</i> , 2011, 49, 592-599. | 1.1 | 6 |
| 5735 | Self-Assembled Conjugated Thiophene-Based Rotaxane Architectures: Structural, Computational, and Spectroscopic Insights into Molecular Aggregation. <i>Advanced Functional Materials</i> , 2011, 21, 834-844. | 7.8 | 24 |
| 5736 | An Alternative Route Towards Metal-Polymer Hybrid Materials Prepared by Vapor-Phase Processing. <i>Advanced Functional Materials</i> , 2011, 21, 3047-3055. | 7.8 | 60 |
| 5737 | Gold versus Silver-Catalyzed Intermolecular Hydroaminations of Alkenes and Dienes. <i>Advanced Synthesis and Catalysis</i> , 2011, 353, 3451-3466. | 2.1 | 44 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5738 | Synthesis, Molecular Structure, and Physical Properties of the Complexes $\{[\text{PhB}(\text{pz})_2(\text{CH}_2\text{SMe})_2]\text{M}\}$ ($\text{M} = \text{Mn}(\text{II}), \text{Fe}(\text{II})$) <i>Tj</i> <i>ET</i> <i>q</i> <i>0</i> <i>0</i> <i>rg</i> <i>BT</i> / <i>Overlo</i> Journal of Inorganic Chemistry, 2011, 2011, 1709-1718. | 1.0 | 59 |
| 5739 | The Flexible Coordination Modes of Guanidine Ligands in Zn Alkyl and Halide Complexes: Chances for Catalysis. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 83-90. | 1.0 | 54 |
| 5740 | Nickel(II) and Cobalt(II) 3-Hydroxy-4-pyridinone Complexes: Synthesis, Characterization and Speciation Studies in Aqueous Solution. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 131-140. | 1.0 | 25 |
| 5741 | Donor-Acceptor Couples and Late Transition Metal Complexes of Oxidation-Labile 1,4,5,8-Tetrakis(guanidino)naphthalene Superbases. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 1593-1604. | 1.0 | 25 |
| 5742 | Substrate Hydroxylation by the Oxido-Iron Intermediate in Aromatic Amino Acid Hydroxylases: A DFT Mechanistic Study. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 2720-2732. | 1.0 | 5 |
| 5743 | From <i>tert</i> -Butylhydrazine Adducts of AlR_3 ($\text{R} = \text{Me}, \text{CMe}_3$) to Oligonuclear Al ₃ Cage Compounds – Evidence for a Hydrazine Twist Across an Al ₃ Triangle. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 1733-1743. | 1.0 | 13 |
| 5744 | ²⁹ Si NMR Shielding Calculations Employing Density Functional Theory, Focussing on Hypervalent Silicon Compounds. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 3365-3373. | 1.0 | 12 |
| 5745 | 1,2-Carbagerma-closo-dodecaborate as a Germanium Ligand in Coordination Chemistry - Synthesis, Structure and Reactivity. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 3349-3356. | 1.0 | 7 |
| 5746 | An Ionic Liquid Designed for Coordination Chemistry Revisited: Synthetic Routes and Safety Tests for 1-Ethyl-3-methylimidazolium Perchlorate ($[\text{emim}][\text{ClO}_4]$). <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 4862-4868. | 1.0 | 15 |
| 5747 | 1,3,2-Diselenaborolanes with an Annelated Dicarba-closo-dodecaborane(12) Unit: Synthesis, Molecular Structure and Reactivity. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 4481-4492. | 1.0 | 12 |
| 5748 | How Important Is Backbonding in Metal Complexes Containing N-Heterocyclic Carbenes? Structural and NBO Analysis. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 5025-5035. | 1.0 | 80 |
| 5749 | The Effect of Strain on the Rh ^I -Catalyzed Rearrangement of Allylamines. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 553-561. | 1.2 | 3 |
| 5750 | Synthesis and Preferred Conformations of All Regio- and Diastereoisomeric Methyl 2,3-Fluorohydroxyalkanoates. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 355-363. | 1.2 | 11 |
| 5751 | New Umpolung Catalysts: Reactivity and Selectivity of Terpenol-Based Lithium Phosphonates in Enantioselective Benzoin-Type Couplings. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 256-263. | 1.2 | 18 |
| 5752 | Regiolone and Isosclerone, Two Enantiomeric Phytotoxic Naphthalenone Pentaketides: Computational Assignment of Absolute Configuration and Its Relationship with Phytotoxic Activity. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 5564-5570. | 1.2 | 60 |
| 5753 | How Space-Filling Is a Pyridine Lone Pair?. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 6725-6731. | 1.2 | 7 |
| 5754 | Theoretical Study of ¹³ C Chemical Shifts Structures of Some <i>ortho</i> -Substituted 3-Anilino-2-nitrobenzo[<i>b</i>]thiophenes and 2-Anilino-3-nitrobenzo[<i>b</i>]thiophenes and Comparison with Experimental. <i>Chinese Journal of Chemistry</i> , 2011, 29, 237-242. | 2.6 | 0 |
| 5755 | Gauge invariant atomic orbital-density functional theory prediction of accurate gas phase ¹ H and ¹³ C NMR chemical shifts. <i>Concepts in Magnetic Resonance Part A: Bridging Education and Research</i> , 2011, 38A, 269-279. | 0.2 | 25 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5756 | Chemical Shift Tensors in Isomers of Adenine: Relation to Aromaticity of Purine Rings?. ChemPhysChem, 2011, 12, 379-388. | 1.0 | 22 |
| 5757 | Chirality Measures for Vectors, Matrices, Operators and Functions. ChemPhysChem, 2011, 12, 197-205. | 1.0 | 18 |
| 5758 | Hydrogen Motion in Proton Sponge Cations: A Theoretical Study. ChemPhysChem, 2011, 12, 1118-1129. | 1.0 | 18 |
| 5759 | On the Photophysics of 1,6-Diphenyl-1,3,5-Hexatriene Isomers and Rotamers. ChemPhysChem, 2011, 12, 1872-1879. | 1.0 | 10 |
| 5760 | On the Importance of the Dispersion Energy for the Thermodynamic Stability of Molecules. ChemPhysChem, 2011, 12, 1258-1261. | 1.0 | 188 |
| 5761 | Spin-Orbit Coupling in Phosphorescent Iridium(III) Complexes. ChemPhysChem, 2011, 12, 2429-2438. | 1.0 | 73 |
| 5762 | Computation of Hyperfine Tensors for Dinuclear Mn ^{III} Mn ^{IV} Complexes by Broken-Symmetry Approaches: Anisotropy Transfer Induced by Local Zero-Field Splitting. ChemPhysChem, 2011, 12, 3170-3179. | 1.0 | 24 |
| 5763 | Theoretical Study of the Photochemistry of a Reversible Three-State Bis-Thioxanthylidene Molecular Switch. ChemPhysChem, 2011, 12, 3348-3353. | 1.0 | 9 |
| 5764 | Ultrafast Dynamics of UV-Excited Imidazole. ChemPhysChem, 2011, 12, 3365-3375. | 1.0 | 33 |
| 5765 | The Role of the π -Linker in Donor-Acceptor Organic Dyes for High-Performance Sensitized Solar Cells. ChemPhysChem, 2011, 12, 2979-2988. | 1.0 | 42 |
| 5766 | The Resonance Raman Spectra of Spheroidene Revisited with a First-Principles Approach. ChemPhysChem, 2011, 12, 3157-3169. | 1.0 | 8 |
| 5767 | Coupled-Cluster Calculations of Vibrational Raman Optical Activity Spectra. ChemPhysChem, 2011, 12, 3442-3448. | 1.0 | 34 |
| 5768 | Vibrational Circular Dichroism: A Valuable Tool for Conformational Analysis and Absolute Configuration Assignment of Chiral 1-Aryl-2,2-Trifluoroethanols. ChemPhysChem, 2011, 12, 3519-3523. | 1.0 | 10 |
| 5769 | Benchmarking Density Functional Methods against the S66 and S66x8 Datasets for Non-Covalent Interactions. ChemPhysChem, 2011, 12, 3421-3433. | 1.0 | 283 |
| 5770 | Transformation of Nickelalactones to Methyl Acrylate: On the Way to a Catalytic Conversion of Carbon Dioxide. ChemSusChem, 2011, 4, 1275-1279. | 3.6 | 59 |
| 5771 | Density functional theory investigation of Cu(I)- and Cu(II)-curcumin complexes. Journal of Computational Chemistry, 2011, 32, 429-438. | 1.5 | 22 |
| 5772 | A reoptimized GROMOS force field for hexopyranose-based carbohydrates accounting for the relative free energies of ring conformers, anomers, epimers, hydroxymethyl rotamers, and glycosidic linkage conformers. Journal of Computational Chemistry, 2011, 32, 998-1032. | 1.5 | 147 |
| 5773 | Shared-memory parallelization of the TURBOMOLE programs AOFORCE, ESCF, and EGRAD: How to quickly parallelize legacy code. Journal of Computational Chemistry, 2011, 32, 1195-1201. | 1.5 | 55 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5774 | Three-dimensional visualization of the first hyperpolarizability tensor. <i>Journal of Computational Chemistry</i> , 2011, 32, 1128-1134. | 1.5 | 62 |
| 5775 | Cyclooctatetraene dianion—an artifact?. <i>Journal of Computational Chemistry</i> , 2011, 32, 1441-1448. | 1.5 | 17 |
| 5776 | Theoretical mechanistic study on the reaction of CN radical with HNCN. <i>Journal of Computational Chemistry</i> , 2011, 32, 1449-1455. | 1.5 | 3 |
| 5777 | Performance of six functionals (LDA, PBE, PBESOL, B3LYP, PBE0, and WC1LYP) in the simulation of vibrational and dielectric properties of crystalline compounds. The case of forsterite Mg_2SiO_4 . <i>Journal of Computational Chemistry</i> , 2011, 32, 1775-1784. | 1.5 | 112 |
| 5778 | Effect of the damping function in dispersion corrected density functional theory. <i>Journal of Computational Chemistry</i> , 2011, 32, 1456-1465. | 1.5 | 15,980 |
| 5779 | SSC: A tool for constructing libraries for systematic screening of conformers. <i>Journal of Computational Chemistry</i> , 2011, 32, 2047-2054. | 1.5 | 7 |
| 5780 | Role of nonlocal exchange in molecular crystals: The case of two proton-ordered phases of ice. <i>Journal of Computational Chemistry</i> , 2011, 32, 2177-2185. | 1.5 | 16 |
| 5781 | A dissected ring current model for assessing magnetic aromaticity: A general approach for both organic and inorganic rings. <i>Journal of Computational Chemistry</i> , 2011, 32, 2422-2431. | 1.5 | 61 |
| 5782 | A computational study of unique properties of pillar[5]quinones: Self-assembly to tubular structures and potential applications as electron acceptors and anion recognizers. <i>Journal of Computational Chemistry</i> , 2011, 32, 2716-2726. | 1.5 | 30 |
| 5783 | Density functional study of neutral and anionic AlO_n and ScO_n with high oxygen content. <i>Journal of Computational Chemistry</i> , 2011, 32, 2974-2982. | 1.5 | 21 |
| 5784 | Theoretical study on the molecular structures of X^+ , L^+ , and L^2 types of lithium phthalocyanine dimer. <i>Journal of Computational Chemistry</i> , 2011, 32, 3062-3067. | 1.5 | 15 |
| 5785 | The coupling constant polarizability and hyperpolarizability of $^{13}C(NH)$ in ^{13}C -methylacetamide, and its application for the multipole spin-spin coupling constant polarizability/reaction field approach to solvation. <i>Journal of Computational Chemistry</i> , 2011, 32, 3168-3174. | 1.5 | 4 |
| 5786 | Kinetic isotope effects calculated with the instanton method. <i>Journal of Computational Chemistry</i> , 2011, 32, 3456-3463. | 1.5 | 35 |
| 5793 | Tuning the Basicity of Ionic Liquids for Equimolar CO_2 Capture. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 4918-4922. | 7.2 | 587 |
| 5794 | Hierarchical Selectivity in Fullerenes: Site-, Regio-, Diastereo-, and Enantiocontrol of the 1,3-Dipolar Cycloaddition to C_{70} . <i>Angewandte Chemie - International Edition</i> , 2011, 50, 6060-6064. | 7.2 | 80 |
| 5795 | Preparation and Characterization of the Binary Group-13 Azides $M(N_3)_3$ and $M(N_3)_3 \cdot nCH_3CN$ ($M=Ga, In, Tl$), $[Ga(N_3)_5]^{2-}$, and $[M(N_3)_6]^{3-}$ ($M=In, Tl$). <i>Angewandte Chemie - International Edition</i> , 2011, 50, 8828-8833. | 7.2 | 27 |
| 5796 | Highly Enantioselective and Efficient Asymmetric Epoxidation Catalysts: Inorganic Nanosheets Modified with α -Amino Acids as Ligands. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 9171-9176. | 7.2 | 63 |
| 5797 | Optical Coupling Between Chiral Biomolecules and Semiconductor Nanoparticles: Size-Dependent Circular Dichroism Absorption. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 11456-11459. | 7.2 | 126 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5798 | Electron-Accepting 6,12-Diethynylindeno[1,2-b]fluorenes: Synthesis, Crystal Structures, and Photophysical Properties. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 11103-11106. | 7.2 | 157 |
| 5799 | β - and γ -Lactams through Palladium-Catalyzed Intramolecular Allylic Alkylation: Enantioselective Synthesis, NMR Investigation, and DFT Rationalization. <i>Chemistry - A European Journal</i> , 2011, 17, 2885-2896. | 1.7 | 36 |
| 5800 | Interfacial Impregnation Chemistry in the Synthesis of Nickel Catalysts Supported on Titania. <i>Chemistry - A European Journal</i> , 2011, 17, 1201-1213. | 1.7 | 13 |
| 5801 | Enhanced Functionality for Donor-Acceptor Oligothiophenes by means of Inclusion of BODIPY: Synthesis, Electrochemistry, Photophysics, and Model Chemistry. <i>Chemistry - A European Journal</i> , 2011, 17, 498-507. | 1.7 | 63 |
| 5802 | Synthesis and Reactivity of 4,5-[1,2-Dicarba-clo-dodecaborano(12)]-1,3-diselenacyclopentane: Opening of the Icosahedron to Give a Zwitterionic Intermediate and Conversion into 7,8-Dicarba-nido-undecaborate(1 ⁻). <i>Chemistry - A European Journal</i> , 2011, 17, 3238-3251. | 1.7 | 21 |
| 5803 | Formation of the Iron-Oxo Hydroxylating Species in the Catalytic Cycle of Aromatic Amino Acid Hydroxylases. <i>Chemistry - A European Journal</i> , 2011, 17, 3746-3758. | 1.7 | 12 |
| 5804 | Solvent-Polarity-Tunable Dimeric Association of a Fullerene (C ₆₀)-N,N-Dimethylaminoazobenzene Dyad: Modulated Electronic Coupling of the Azo Chromophore with a Substituted 3D Fullerene. <i>Chemistry - A European Journal</i> , 2011, 17, 5327-5343. | 1.7 | 19 |
| 5805 | Quantum Chemical Studies of the Hydration of Sr ²⁺ in Vacuum and Aqueous Solution. <i>Chemistry - A European Journal</i> , 2011, 17, 5060-5067. | 1.7 | 17 |
| 5806 | Uncommon Coordination Behaviour of P(S) and P(Se) Units when Bonded to Carboranyl Clusters: Experimental and Computational Studies on the Oxidation of Carboranyl Phosphine Ligands. <i>Chemistry - A European Journal</i> , 2011, 17, 4429-4443. | 1.7 | 37 |
| 5807 | Analysis of Tertiary Phosphanes, Arsanes, and Stibanes as Bridging Ligands in Dinuclear Group ⁹ Complexes. <i>Chemistry - A European Journal</i> , 2011, 17, 7228-7235. | 1.7 | 8 |
| 5808 | Probing Lipid Peroxidation by Using Linoleic Acid and Benzophenone. <i>Chemistry - A European Journal</i> , 2011, 17, 10089-10096. | 1.7 | 10 |
| 5809 | Pt ^{II} Coordination to N1 of 9-Methylguanine: Why it Facilitates Binding of Additional Metal Ions to the Purine Ring. <i>Chemistry - A European Journal</i> , 2011, 17, 9970-9983. | 1.7 | 14 |
| 5810 | Neutral Nickel Oligo- and Polymerization Catalysts: The Importance of Alkyl Phosphine Intermediates in Chain Termination. <i>Chemistry - A European Journal</i> , 2011, 17, 14628-14642. | 1.7 | 16 |
| 5811 | Gold-Catalyzed, Intramolecular, Oxygen-Transfer Reactions of 2-Alkynyl-1,5-diketones or 2-Alkynyl-5-ketoesters: Scope, Expansion, and Mechanistic Investigations on a New [4+2] Cycloaddition. <i>Chemistry - A European Journal</i> , 2011, 17, 10690-10699. | 1.7 | 17 |
| 5812 | Binap-Gold(I) versus Binap-Silver Trifluoroacetate Complexes as Catalysts in 1,3-Dipolar Cycloadditions of Azomethine Ylides. <i>Chemistry - A European Journal</i> , 2011, 17, 14224-14233. | 1.7 | 45 |
| 5813 | Nature of the Intermediates in Gold(I)-Catalyzed Cyclizations of 1,5-Enynes. <i>Chemistry - A European Journal</i> , 2011, 17, 10972-10978. | 1.7 | 82 |
| 5814 | Intramolecular [2+2+2] Cycloaddition Reactions of Yne-cyne and Yne-cyne-ene Ene-diyne Catalysed by Rh ^I : Experimental and Theoretical Mechanistic Studies. <i>Chemistry - A European Journal</i> , 2011, 17, 14493-14507. | 1.7 | 32 |
| 5815 | Molecular dynamics study of selective adsorption of PCB on activated carbon. <i>Fluid Phase Equilibria</i> , 2011, 307, 58-65. | 1.4 | 11 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5816 | Î±-Tocopherol impact on oxy-radical induced free radical decomposition of DMSO: Spin trapping EPR and theoretical studies. <i>Chemical Physics</i> , 2011, 383, 27-34. | 0.9 | 15 |
| 5817 | Pharmacophore models based studies on the affinity and selectivity toward 5-HT1A with reference to Î±1-adrenergic receptors among arylpiperazine derivatives of phenytoin. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 1349-1360. | 1.4 | 23 |
| 5818 | Design of small molecule inhibitors of acetyl-CoA carboxylase 1 and 2 showing reduction of hepatic malonyl-CoA levels in vivo in obese Zucker rats. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 3039-3053. | 1.4 | 27 |
| 5819 | Requirements for mammalian carboxylesterase inhibition by substituted ethane-1,2-diones. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 4635-4643. | 1.4 | 20 |
| 5820 | The effect of SiC substrate microstructure and impurities on the phase formation in carbide-derived carbon. <i>Carbon</i> , 2011, 49, 1189-1198. | 5.4 | 10 |
| 5821 | A combined theoretical and spectroscopic study of 4,6-di-O-acetyl-2,3-dideoxy-d-erythro-hex-2-enopyranosyl sulfamide: a novel glycosyl carbonic anhydrase IX inhibitor. <i>Carbohydrate Research</i> , 2011, 346, 442-448. | 1.1 | 8 |
| 5822 | Direct esterification of p-nitrobenzoic acid with n-butanol using diethyl chlorophosphate in pyridine: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 13-17. | 1.1 | 11 |
| 5823 | A through-space charge transfer mechanism for explaining the oxidation of 2-chlorophenol on a tetrasulphonated nickel(III) phthalocyanine. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 161-167. | 1.1 | 6 |
| 5824 | Quantum chemical and RRKM/master equation studies of cyclopropene ozonolysis. <i>Computational and Theoretical Chemistry</i> , 2011, 965, 305-312. | 1.1 | 13 |
| 5825 | Effects of the self-interaction error in Kohn-Sham calculations: A DFT+U case study on penta-aqua uranyl(VI). <i>Computational and Theoretical Chemistry</i> , 2011, 963, 337-343. | 1.1 | 12 |
| 5826 | Similarity analysis of the conformational potential energy surface of n-pentane. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 378-383. | 1.1 | 9 |
| 5827 | Computational studies on Schiff-base formation: Implications for the catalytic mechanism of porphobilinogen synthase. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 479-489. | 1.1 | 24 |
| 5828 | Deprotonation studies of Cu+â€“guanine and Cu2+â€“guanine complexes by theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 490-496. | 1.1 | 5 |
| 5829 | Theoretical investigation of thermal activation of methane by [Pd(H)(OH)]+. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 470-474. | 1.1 | 4 |
| 5830 | Theoretical study on structures and properties of lantern-like compounds derived from ammonia borane. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 510-516. | 1.1 | 1 |
| 5831 | How does the nonlocal HF exchange influence the electron excitation of Bacteriochlorophyll and its assembly. <i>Computational and Theoretical Chemistry</i> , 2011, 965, 53-59. | 1.1 | 12 |
| 5832 | Theoretical study on the reaction mechanism of +SCX (X=O, S). <i>Computational and Theoretical Chemistry</i> , 2011, 965, 221-230. | 1.1 | 0 |
| 5833 | Hydrogen bond cooperativity in polyols: A DFT and AIM study. <i>Computational and Theoretical Chemistry</i> , 2011, 967, 12-18. | 1.1 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5834 | A DFT study of two-state reactivity on the reaction of N ₂ O with Sc ⁺ in the gas phase. Computational and Theoretical Chemistry, 2011, 966, 352-356. | 1.1 | 1 |
| 5835 | Theoretical studies on the isomers and tautomers of 22-membered macrocyclic ligand. Computational and Theoretical Chemistry, 2011, 967, 75-80. | 1.1 | 1 |
| 5836 | Assessment of DFT functionals for the calculation of interaction-induced electric properties of molecular complexes. Chemical Physics Letters, 2011, 503, 39-44. | 1.2 | 14 |
| 5837 | NMR study of a phasmid-like liquid crystal. Chemical Physics Letters, 2011, 507, 96-99. | 1.2 | 6 |
| 5838 | W4-11: A high-confidence benchmark dataset for computational thermochemistry derived from first-principles W4 data. Chemical Physics Letters, 2011, 510, 165-178. | 1.2 | 353 |
| 5839 | Effect of aromatization of the ring on intramolecular H-bond in 3-hydroxy-4-formyl derivatives of fulvene. Chemical Physics Letters, 2011, 510, 53-56. | 1.2 | 18 |
| 5840 | N-Heteroaryl-1,8-naphthalimide fluorescent sensor for water: Molecular design, synthesis and properties. Dyes and Pigments, 2011, 88, 307-314. | 2.0 | 109 |
| 5841 | Density functional theory study of the electron spectra of formamide vapor. Journal of Electron Spectroscopy and Related Phenomena, 2011, 184, 164-169. | 0.8 | 16 |
| 5842 | Vibrational and NMR properties of polyynes. Carbon, 2011, 49, 3340-3345. | 5.4 | 11 |
| 5843 | Novel heterometallic palladium-silver complex. Inorganica Chimica Acta, 2011, 370, 382-387. | 1.2 | 29 |
| 5844 | Proper and improper aminoketyl radicals in electron-based peptide dissociations. International Journal of Mass Spectrometry, 2011, 301, 55-61. | 0.7 | 30 |
| 5845 | Electron ionization and gas-phase ion molecule reactions of methylcyclohexane. International Journal of Mass Spectrometry, 2011, 300, 2-11. | 0.7 | 3 |
| 5846 | A combined theoretical and experimental study of mechanisms of fragmentation active for PHB oligomers in negative-ion mode multistage mass spectrometry. International Journal of Mass Spectrometry, 2011, 304, 15-24. | 0.7 | 9 |
| 5847 | Phosphonic drugs: Experimental and theoretical spectroscopic studies of fosfomycin. Journal of Molecular Structure, 2011, 986, 49-56. | 1.8 | 12 |
| 5848 | Spectral characterization and crystal structure of tetrahydropyran-4-one thiosemicarbazones. Journal of Molecular Structure, 2011, 989, 1-9. | 1.8 | 5 |
| 5849 | Synthesis, spectroscopic characterization, calculational studies and in vitro antitumoral activity of 4-(3-(1H-imidazol-1-yl)propyl)-(thiophen-2-ylmethyl)-1H-1,2,4-triazol-5(4H)-one. Journal of Molecular Structure, 2011, 989, 101-108. | 1.8 | 11 |
| 5850 | Structure and spectroscopic properties of bis(1-carboxyethyl-3-aminopyridinium) hydrobromide monohydrate. Journal of Molecular Structure, 2011, 994, 13-20. | 1.8 | 7 |
| 5851 | FT-IR, FT-Raman spectroscopy and computational study of | | |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5852 | Raman experimental and DFT theoretical studies on the adsorption behavior of MHBA on silver nanoparticles. <i>Journal of Molecular Structure</i> , 2011, 998, 49-52. | 1.8 | 4 |
| 5853 | Calculation of solid state molecular ionisation energies and electron affinities for organic semiconductors. <i>Organic Electronics</i> , 2011, 12, 394-403. | 1.4 | 69 |
| 5854 | DFT calculation and AIM-analysis of the substituent influence on the structure of (1-azabuta-1,3-diene)tetracarbonyliron(0) complexes. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 622-631. | 0.8 | 1 |
| 5855 | Computational study of the cyclopalladation mechanism of azobenzene with PdCl ₂ in N,N-dimethylformamide. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 661-669. | 0.8 | 13 |
| 5856 | Room-temperature long-lived [Nb ₂ F ₁₁] ⁺ salts of radical cations of simple arenes: EPR, UV-Vis and DFT results. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 1294-1300. | 0.8 | 18 |
| 5857 | Rhodium(I) complexes with P coordinated phosphinofunctionalized alkyl phenyl sulfide, sulfoxide and sulfone ligands and their reactions with sodium bis(trimethylsilyl)amide and Ag[BF ₄]. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 1768-1781. | 0.8 | 4 |
| 5858 | Synthesis and structure of planar chiral ferroceno[d]pyridazinones, the first representatives of a novel class of fused metallocenes. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 1626-1631. | 0.8 | 10 |
| 5859 | Theoretical investigation of the scope of sequential ligand tuning using a bifunctional scorpionate tris(1,2,4-triazolyl)borate-based architecture. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 2580-2583. | 0.8 | 3 |
| 5860 | Elucidation of the mechanism of single-stranded DNA interaction with methylene blue: A spectroscopic approach. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2011, 218, 26-32. | 2.0 | 56 |
| 5861 | The effect of constitutional and conformational isomerization on the electrical properties of diblock molecular diode. <i>Organic Electronics</i> , 2011, 12, 1080-1092. | 1.4 | 11 |
| 5862 | Capturing the spin state diversity of iron(III)-aryl porphyrins: OLYP is better than TPSSh. <i>Journal of Inorganic Biochemistry</i> , 2011, 105, 84-91. | 1.5 | 40 |
| 5863 | Experimental and computational study on the energetics of 10,11-dihydro-5H-dibenzo[a,d]cycloheptene (dibenzosuberane). <i>Journal of Chemical Thermodynamics</i> , 2011, 43, 364-370. | 1.0 | 8 |
| 5864 | EPR study of gamma irradiated 2,5-di-tert-butyl-hydroquinone single crystals. <i>Radiation Physics and Chemistry</i> , 2011, 80, 38-43. | 1.4 | 18 |
| 5865 | EPR study of gamma-irradiated amphi-phenylglyoxime single crystals. <i>Radiation Physics and Chemistry</i> , 2011, 80, 742-749. | 1.4 | 8 |
| 5866 | Structural studies and anticancer activity of a novel (N ₆ O ₄) macrocyclic ligand and its Cu(II) complexes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 78, 360-370. | 2.0 | 71 |
| 5867 | Experimental and theoretical studies on the identification of p-biphenyloxycarbonylphenyl acrylate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 1024-1033. | 2.0 | 15 |
| 5868 | FT-IR, FT-Raman spectroscopy and computational study of (E)-4-((anthracen-9-ylmethylene)amino)-N-carbamimidoylbenzene sulfonamide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 1584-1592. | 2.0 | 42 |
| 5869 | Stoichiometric aryl nitrile formation from amides and aroyl isocyanates using high-valent early transition metal complexes and a catalytic process from the aroyl isocyanates. <i>Polyhedron</i> , 2011, 30, 632-637. | 1.0 | 23 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5870 | Axial ligand influence on geometries, charge distributions and electronic structures of iron tetraazamacrocyclic [Fe(II)TIM(X)(Y)] ²⁺ complexes assessed by Density Functional Theory. <i>Polyhedron</i> , 2011, 30, 1396-1403. | 1.0 | 2 |
| 5871 | Synthesis, chemical characterization and preliminary in vitro antitumor activity evaluation of new ruthenium(II) complexes with sugar derivatives. <i>Polyhedron</i> , 2011, 30, 1671-1679. | 1.0 | 5 |
| 5872 | Design of new benzothiadiazole-based linear and star molecules with different functional groups as solar cells materials: A theoretical approach. <i>Solar Energy Materials and Solar Cells</i> , 2011, 95, 1800-1810. | 3.0 | 33 |
| 5873 | Study on medium ring heterocycles: synthesis and structure of novel condensed pyrazolo[1,4]diazocinones including single enantiomers. <i>Tetrahedron</i> , 2011, 67, 2979-2990. | 1.0 | 8 |
| 5874 | Three-component conformational equilibria of some flexible pyrrolidin-2-(thi)ones in solution by NMR data (¹³ C, ¹ H, and nJHH) and their DFT predictions: a confrontation of different approaches. <i>Tetrahedron</i> , 2011, 67, 6901-6916. | 1.0 | 16 |
| 5875 | Chiral phosphine-phosphite ligands in the enantioselective 1,4-addition of Grignard reagents to $\hat{1}\pm, \hat{1}^2$ -unsaturated carbonyl compounds. <i>Tetrahedron: Asymmetry</i> , 2011, 22, 887-892. | 1.8 | 52 |
| 5876 | S-arylation of mercaptobenzimidazoles using Cu(I) catalysts—experimental and theoretical observations. <i>Tetrahedron Letters</i> , 2011, 52, 3347-3352. | 0.7 | 29 |
| 5877 | Inelastic Neutron Scattering (INS) Study of Low Frequency Vibrations and Hydrogen Bonding of (<i>E</i>)-2-Hydroxyimino-2-Cyanoacetic Acid Ethyl Ester. <i>Zeitschrift Fur Physikalische Chemie</i> , 2011, 225, 183-216. | 1.4 | 1 |
| 5878 | First-principles study of ⁷⁵ As NQR in arsenic-chalcogenide compounds. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 055502. | 0.7 | 1 |
| 5879 | Density Functional Theory Study on the Interaction of O ₂ Molecule with Cobalt(6)Pyrrole Clusters. <i>Japanese Journal of Applied Physics</i> , 2011, 50, 055702. | 0.8 | 8 |
| 5880 | Photodissociation and Density Functional Calculations of Small V _m O _n Clusters. <i>Chinese Journal of Chemical Physics</i> , 2011, 24, 572-579. | 0.6 | 10 |
| 5881 | Scalable implementations of accurate excited-state coupled cluster theories. , 2011, , . | | 24 |
| 5882 | Cr(CO) ₆ photochemistry: Semi-classical study of UV absorption spectral intensities and dynamics of photodissociation. <i>Journal of Chemical Physics</i> , 2011, 134, 164305. | 1.2 | 28 |
| 5883 | Application of an efficient multireference approach to free-base porphyrin and metalloporphyrins: Ground, excited, and positive ion states. <i>Journal of Chemical Physics</i> , 2011, 135, 084118. | 1.2 | 16 |
| 5884 | Electric field effects on nuclear magnetic shielding of the 1:1 and 2:1 (homo and heterochiral) complexes of XOOX ² (X, X ² = H, CH ₃) with lithium cation and their chiral discrimination. <i>Journal of Chemical Physics</i> , 2011, 135, 104116. | 1.2 | 9 |
| 5885 | Photoelectron spectroscopy of higher bromine and iodine oxide anions: Electron affinities and electronic structures of BrO _{2,3} and IO ₂ ⁴ radicals. <i>Journal of Chemical Physics</i> , 2011, 135, 184309. | 1.2 | 13 |
| 5886 | Flickering dipoles in the gas phase: Structures, internal dynamics, and dipole moments of $\hat{1}^2$ -naphthol-H ₂ O in its ground and excited electronic states. <i>Journal of Chemical Physics</i> , 2011, 134, 114304. | 1.2 | 9 |
| 5887 | Optical and phonon excitations of modified Pandey chains at the Si(111)-2 \times 1 surface. <i>Physical Review B</i> , 2011, 84, . | 1.1 | 11 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5888 | Improved lattice constants, surface energies, and CO desorption energies from a semilocal density functional. <i>Physical Review B</i> , 2011, 83, . | 1.1 | 67 |
| 5889 | Dibromido[(S,S)-ethylenediamine-N,N ^ε -di-(3-cyclohexyl)propanoato]platinum(IV): synthesis, characterization, and DFT calculations. <i>Journal of Coordination Chemistry</i> , 2011, 64, 1016-1022. | 0.8 | 2 |
| 5890 | Importance of anisotropy in the evaluation of dispersion interactions. <i>Physical Review A</i> , 2011, 83, . | 1.0 | 16 |
| 5891 | Density functional theory investigation of conformations, C_{13} shielding, and magnetic field interactions in a V-shaped phenylene bis carboxylate homologous series. <i>Physical Review E</i> , 2011, 83, 041712. | 0.8 | 8 |
| 5892 | Circularly polarized photoluminescence from platinum porphyrins in organic hosts: Magnetic field and temperature dependence. <i>Journal of Applied Physics</i> , 2011, 109, . | 1.1 | 13 |
| 5893 | Density functional study of multiplicity-changing valence and Rydberg excitations of p-block elements: Delta self-consistent field, collinear spin-flip time-dependent density functional theory (DFT), and conventional time-dependent DFT. <i>Journal of Chemical Physics</i> , 2011, 135, 044118. | 1.2 | 57 |
| 5894 | On the interaction between supercritical CO ₂ and epoxides combining infrared absorption spectroscopy and quantum chemistry calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 9209. | 1.3 | 15 |
| 5895 | Communication: A global hybrid generalized gradient approximation to the exchange-correlation functional that satisfies the second-order density-gradient constraint and has broad applicability in chemistry. <i>Journal of Chemical Physics</i> , 2011, 135, 191102. | 1.2 | 254 |
| 5896 | How Flexible are DNA Constituents? The Quantum-Mechanical Study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2011, 29, 563-575. | 2.0 | 51 |
| 5897 | van der Waals density functional study of energetic, structural, and vibrational properties of small water clusters and ice I_h h_{46} . <i>Physical Review B</i> , 2011, 84, . | 1.1 | 46 |
| 5898 | Self-assembled cyclic oligothiophene nanotubes: Electronic properties from a dispersion-corrected hybrid functional. <i>Physical Review B</i> , 2011, 84, . | 1.1 | 30 |
| 5899 | Spectroscopic and computational studies of matrix-isolated iso-CHBr ₃ : Structure, properties, and photochemistry of iso-bromoform. <i>Journal of Chemical Physics</i> , 2011, 135, 124503. | 1.2 | 24 |
| 5900 | A classical molecular dynamics study of a Diels Alder cycloaddition in supercritical water. <i>Molecular Physics</i> , 2011, 109, 773-781. | 0.8 | 2 |
| 5902 | Theoretical Investigation on the Structure and Optical Properties of Alq ₃ and its Difluorinated Derivatives. <i>Advanced Materials Research</i> , 2011, 287-290, 1526-1531. | 0.3 | 1 |
| 5903 | Correlating computational docking predictions with Raman spectroscopy for β -lactoglobulin-porphyrin complexes. , 2011, , . | | 0 |
| 5904 | Nanocatalyst structure as a template to define chirality of nascent single-walled carbon nanotubes. <i>Journal of Chemical Physics</i> , 2011, 134, 014705. | 1.2 | 36 |
| 5905 | Photoelectron and computational studies of the copper-nucleoside anionic complexes, Cu ^ε (cytidine) and Cu ^ε (uridine). <i>Journal of Chemical Physics</i> , 2011, 134, 054318. | 1.2 | 2 |
| 5906 | A fast doubly hybrid density functional method close to chemical accuracy using a local opposite spin ansatz. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 19896-19900. | 3.3 | 143 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5907 | Comparing modern density functionals for conjugated polymer band structures: Screened hybrid, Minnesota, and Rung 3.5 approximations. <i>Journal of Chemical Physics</i> , 2011, 134, 184105. | 1.2 | 46 |
| 5908 | Chemistry of defect induced photoluminescence in chalcopyrites: The case of CuAlS ₂ . <i>Journal of Applied Physics</i> , 2011, 109, . | 1.1 | 35 |
| 5909 | Development and application of the analytical energy gradient for the normalized elimination of the small component method. <i>Journal of Chemical Physics</i> , 2011, 134, 244117. | 1.2 | 68 |
| 5910 | Implementation of screened hybrid density functional for periodic systems with numerical atomic orbitals: Basis function fitting and integral screening. <i>Journal of Chemical Physics</i> , 2011, 135, 034110. | 1.2 | 24 |
| 5911 | On the formation of hydrogen gas on copper in anoxic water. <i>Journal of Chemical Physics</i> , 2011, 135, 084709. | 1.2 | 24 |
| 5912 | A DFT STUDY ON CO INSERTION AND C^{C} REDUCTIVE ELIMINATION INVOLVED IN THE CARBONYLATION OF METALLACYCLIC ZIRCONACENES. <i>Journal of Theoretical and Computational Chemistry</i> , 2011, 10, 9-17. | 1.8 | 0 |
| 5913 | DENSITY FUNCTIONAL THEORY INVESTIGATE OF THE RgFn (Rg = Kr, Xe; n = 2,4,6) MOLECULES. <i>International Journal of Modern Physics C</i> , 2011, 22, 155-167. | 0.8 | 1 |
| 5914 | Communication: Tailoring the optical gap in light-harvesting molecules. <i>Journal of Chemical Physics</i> , 2011, 134, 151101. | 1.2 | 109 |
| 5915 | Unusual mechanism for H ₃ ⁺ formation from ethane as obtained by femtosecond laser pulse ionization and quantum chemical calculations. <i>Journal of Chemical Physics</i> , 2011, 134, 114302. | 1.2 | 51 |
| 5916 | Electron transfer dissociation of a melectin peptide: correlating the precursor ion structure with peptide backbone dissociations. <i>Collection of Czechoslovak Chemical Communications</i> , 2011, 76, 295-309. | 1.0 | 7 |
| 5917 | Reconsidering an analytical gradient expression within a divide-and-conquer self-consistent field approach: Exact formula and its approximate treatment. <i>Journal of Chemical Physics</i> , 2011, 134, 034105. | 1.2 | 45 |
| 5918 | Quantum chemical assessment of the binding energy of CuO ⁺ . <i>Journal of Chemical Physics</i> , 2011, 134, 064304. | 1.2 | 36 |
| 5919 | Benchmarking the multipole shielding polarizability/reaction field approach to solvation against QM/MM: Applications to the shielding constants of N-methylacetamide. <i>Journal of Chemical Physics</i> , 2011, 134, 044514. | 1.2 | 9 |
| 5920 | Novel pentagonal silicon rings and nanowheels stabilized by flat pentacoordinate carbon(s). <i>Journal of Chemical Physics</i> , 2011, 134, 094312. | 1.2 | 11 |
| 5921 | An efficient, fragment-based electronic structure method for molecular systems: Self-consistent polarization with perturbative two-body exchange and dispersion. <i>Journal of Chemical Physics</i> , 2011, 134, 094118. | 1.2 | 82 |
| 5922 | Gauge-origin independent calculations of Jones birefringence. <i>Journal of Chemical Physics</i> , 2011, 135, 134114. | 1.2 | 8 |
| 5923 | CAN NEUTRAL AND IONIZED POLYCYCLIC AROMATIC HYDROCARBONS BE CARRIERS OF THE ULTRAVIOLET EXTINCTION BUMP AND THE DIFFUSE INTERSTELLAR BANDS?. <i>Astrophysical Journal</i> , 2011, 742, 2. | 1.6 | 57 |
| 5924 | Theoretical Investigation on the PCP(O) Linear Moiety: How to Stabilize Diphosphaallenic Derivatives. Phosphorus, Sulfur and Silicon and the Related Elements, 2011, 186, 2321-2331. | 0.8 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5925 | Assessment of correlation energies based on the random-phase approximation. <i>New Journal of Physics</i> , 2012, 14, 043002. | 1.2 | 137 |
| 5926 | Experimental and Modeling Studies of the Oxidation of Surrogate Bio-Aviation Fuels. <i>Journal of Engineering for Gas Turbines and Power</i> , 2012, 134, . | 0.5 | 1 |
| 5927 | Calculations of hyperfine coupling constant of the TMPD molecule. <i>Acta Chimica Slovaca</i> , 2012, 5, . | 0.5 | 0 |
| 5928 | Molecular Mechanisms of Pharmaceutical Drug Binding into Calsequestrin. <i>International Journal of Molecular Sciences</i> , 2012, 13, 14326-14343. | 1.8 | 7 |
| 5929 | O ₂ +C ₂ H ₄ potential energy surface: lowest-lying singlet at the multireference level. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1. | 0.5 | 5 |
| 5930 | Non-empirical improvement of PBE and its hybrid PBE0 for general description of molecular properties. <i>Journal of Chemical Physics</i> , 2012, 136, 104108. | 1.2 | 78 |
| 5931 | Transition Metal Catalyzed Enantioselective Allylic Substitution in Organic Synthesis. <i>Topics in Organometallic Chemistry</i> , 2012, , . | 0.7 | 101 |
| 5932 | Electronic excitation spectrum of the photosensitizer [Ir(ppy) ₂ (bpy)] ⁺ . <i>Journal of Chemical Physics</i> , 2012, 136, 214305. | 1.2 | 37 |
| 5933 | Atomic-scale computer simulation of functional materials: methodologies and applications. , 2012, , 643-662e. | | 0 |
| 5934 | Experimental and theoretical investigations on photoabsorption and photoionization of trimethylphosphate in the vacuum-ultraviolet energy range. <i>Journal of Chemical Physics</i> , 2012, 137, 184305. | 1.2 | 7 |
| 5935 | Long-range corrected hybrid meta-generalized-gradient approximations with dispersion corrections. <i>Journal of Chemical Physics</i> , 2012, 136, 154109. | 1.2 | 101 |
| 5936 | Softening of C-H Symmetric Stretching Vibrational Modes for CH ₂ and CH ₃ Radicals Adsorbed on Cu _n (n=1-6) Clusters. <i>Chinese Journal of Chemical Physics</i> , 2012, 25, 649-653. | 0.6 | 0 |
| 5937 | Rovibrational effects on NMR shieldings in a heavy-element system: XeF ₂ . <i>Journal of Chemical Physics</i> , 2012, 137, 214309. | 1.2 | 8 |
| 5938 | Vibrationally resolved photoelectron imaging of platinum carbonyl anion Pt(CO) _n ⁻ (n = 1, 2, 3, 4, 5, 6). <i>Journal of Chemical Physics</i> , 2012, 136, 104108. | 1.2 | 10 |
| 5939 | Importance of the correlation contribution for local hybrid functionals: Range separation and self-interaction corrections. <i>Journal of Chemical Physics</i> , 2012, 136, 014111. | 1.2 | 83 |
| 5940 | Stockholder projector analysis: A Hilbert-space partitioning of the molecular one-electron density matrix with orthogonal projectors. <i>Journal of Chemical Physics</i> , 2012, 136, 014107. | 1.2 | 13 |
| 5941 | Nonspherical model density matrices for Rung 3.5 density functionals. <i>Journal of Chemical Physics</i> , 2012, 136, 024111. | 1.2 | 20 |
| 5942 | Calculation of longitudinal polarizability and second hyperpolarizability of polyacetylene with the coupled perturbed Hartree-Fock/Kohn-Sham scheme: Where it is shown how finite oligomer chains tend to the infinite periodic polymer. <i>Journal of Chemical Physics</i> , 2012, 136, 114101. | 1.2 | 21 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5943 | The optical activity of carvone: A theoretical and experimental investigation. <i>Journal of Chemical Physics</i> , 2012, 136, 114512. | 1.2 | 25 |
| 5944 | Improved constraint satisfaction in a simple generalized gradient approximation exchange functional. <i>Journal of Chemical Physics</i> , 2012, 136, 144115. | 1.2 | 31 |
| 5945 | Effects of intermolecular interaction on the energy distribution of valence electronic states of a carbazole-based material in amorphous thin films. <i>Journal of Chemical Physics</i> , 2012, 136, 204706. | 1.2 | 9 |
| 5946 | On the fundamental processes in molecular electrical doping of organic semiconductors. <i>AIP Conference Proceedings</i> , 2012, , . | 0.3 | 11 |
| 5947 | Analytic calculation of second-order electric response properties with the normalized elimination of the small component (NESC) method. <i>Journal of Chemical Physics</i> , 2012, 137, 084108. | 1.2 | 26 |
| 5948 | High resolution electron energy loss spectroscopy of clean and hydrogen covered Si(001) surfaces: First principles calculations. <i>Journal of Chemical Physics</i> , 2012, 137, 094701. | 1.2 | 1 |
| 5949 | A non-self-consistent range-separated time-dependent density functional approach for large-scale simulations. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 205801. | 0.7 | 20 |
| 5950 | Spin densities from subsystem density-functional theory: Assessment and application to a photosynthetic reaction center complex model. <i>Journal of Chemical Physics</i> , 2012, 136, 194104. | 1.2 | 35 |
| 5951 | Finding Density Functionals with Machine Learning. <i>Physical Review Letters</i> , 2012, 108, 253002. | 2.9 | 495 |
| 5952 | Theoretical investigation of structural stability and electronic properties of hydrogenated silicon nanocrystals: Size, shape, and surface reconstruction. <i>Physical Review B</i> , 2012, 86, . | 1.1 | 11 |
| 5953 | Benchmark study for the application of density functional theory to the prediction of octahedral tilting in perovskites. <i>Physical Review B</i> , 2012, 86, . | 1.1 | 28 |
| 5954 | Vibrational frequencies of anti-diabetic drug studied by terahertz time-domain spectroscopy. <i>Applied Physics Letters</i> , 2012, 100, . | 1.5 | 30 |
| 5955 | Reaction mechanisms for atomic layer deposition of aluminum oxide on semiconductor substrates. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2012, 30, . | 0.9 | 53 |
| 5956 | Portable e-nose based on polymer/CNT sensor array for protein-based detection. , 2012, , . | | 11 |
| 5957 | Potential energy surface for dissociation including spin-orbit effects. <i>Molecular Physics</i> , 2012, 110, 2599-2609. | 0.8 | 6 |
| 5958 | Relating normal vibrational modes to local vibrational modes with the help of an adiabatic connection scheme. <i>Journal of Chemical Physics</i> , 2012, 137, 084114. | 1.2 | 113 |
| 5959 | B80 and B101-103 clusters: Remarkable stability of the core-shell structures established by validated density functionals. <i>Journal of Chemical Physics</i> , 2012, 136, 074302. | 1.2 | 150 |
| 5960 | The effect of the Perdew-Zunger self-interaction correction to density functionals on the energetics of small molecules. <i>Journal of Chemical Physics</i> , 2012, 137, 124102. | 1.2 | 89 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5961 | Synthesis, characterization, and density functional study of some manganese(III) Schiff-base complexes. <i>Journal of Coordination Chemistry</i> , 2012, 65, 980-993. | 0.8 | 8 |
| 5962 | THE GEOMETRIES AND PROTON TRANSFER OF HYDRATED DIVALENT LEAD ION CLUSTERS $[Pb(H_2O)_n]^{2+(n-)} Tj ETQq1 1 0.784314$ | 1.8 | 10 |
| 5963 | High sensitivity, supramolecular thin films for sensing of methane. , 2012, , . | | 0 |
| 5964 | Water exchange on beryllium complexes: part VIII " influence of neutral electron pair donors. <i>Journal of Coordination Chemistry</i> , 2012, 65, 4359-4374. | 0.8 | 4 |
| 5965 | Relativistic Time-Dependent Density Functional Theory and Excited States Calculations for the Zinc Dimer. <i>Journal of Atomic, Molecular, and Optical Physics</i> , 2012, 2012, 1-16. | 0.5 | 1 |
| 5966 | Electrodeposition of Y_2O_3 "Au composite coatings for SOFC interconnects:in situmonitoring of film growth by surface enhanced Raman spectroscopy. <i>Transactions of the Institute of Metal Finishing</i> , 2012, 90, 30-37. | 0.6 | 6 |
| 5967 | GAMESS As a Free Quantum-Mechanical Platform for Drug Research. <i>Current Topics in Medicinal Chemistry</i> , 2012, 12, 2013-2033. | 1.0 | 118 |
| 5968 | Radicals organized by disk shaped aromatics " polymorphism and co-crystals that tune inter-electron exchange. <i>CrystEngComm</i> , 2012, 14, 1515-1526. | 1.3 | 20 |
| 5969 | A DFT Study on the Mechanism of Samarium (II)-catalyzed Cyclopropanation Synthesis with α,β-unsaturated Carboxylic Acids, Alcohols and Amides. <i>Current Organic Chemistry</i> , 2012, 16, 1934-1941. | 0.9 | 0 |
| 5970 | Dynamic hyperpolarizability calculations of large systems: The linear-scaling divide-and-conquer approach. <i>Journal of Chemical Physics</i> , 2012, 136, 084108. | 1.2 | 17 |
| 5971 | Rapid anharmonic vibrational corrections derived from partial Hessian analysis. <i>Journal of Chemical Physics</i> , 2012, 136, 224102. | 1.2 | 20 |
| 5972 | Inelastic Neutron Scattering (INS) Study of Low Frequency Vibrations of Acid K Salt of (E)-2-Hydroxyimino-2-Cyanoacetic Acid Ethyl Ester and its Phase Situation by DSC Method. <i>Zeitschrift Fur Physikalische Chemie</i> , 2012, 226, 291-314. | 1.4 | 1 |
| 5973 | Side-chain degradation of perfluorosulfonic acid membranes: An ab initio study. <i>Journal of Materials Research</i> , 2012, 27, 1982-1991. | 1.2 | 25 |
| 5974 | Effectiveness of Optimizing Geometry for $CaMn_4O_5$ Cluster at 1.9 Å... Resolved OEC and Proposal for Oxidation Mechanism from S0 to S3 States. <i>Chemistry Letters</i> , 2012, 41, 18-20. | 0.7 | 13 |
| 5975 | Oxygen Reduction Reaction on Cobalt"(6)Pyrrole Cluster: Density Functional Theory Study. <i>Journal of the Physical Society of Japan</i> , 2012, 81, 034703. | 0.7 | 15 |
| 5976 | Cyclodextrin effects on the photochromism of spiropyrans/β ² -cyclodextrin inclusion polymers. <i>Materials Chemistry and Physics</i> , 2012, 136, 151-159. | 2.0 | 15 |
| 5977 | Molecular structures of $M_2N_2X_2$ (M and N = B, Al, and Ga) clusters using the gradient embedded genetic algorithm. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14850. | 1.3 | 18 |
| 5978 | Theoretical investigation of the conventional CX_1X_2 (X1, X2=H, F, Cl, Br, and I) compounds. <i>Computational and Theoretical Chemistry</i> , 2012, 997, 1-6. | 1.1 | 0 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 5979 | QM/MM Investigations Of Organic Chemistry Oriented Questions. Topics in Current Chemistry, 2012, 351, 25-101. | 4.0 | 3 |
| 5980 | Why the Standard B3LYP/6-31G* Model Chemistry Should Not Be Used in DFT Calculations of Molecular Thermochemistry: Understanding and Correcting the Problem. Journal of Organic Chemistry, 2012, 77, 10824-10834. | 1.7 | 407 |
| 5981 | A geometrical correction for the inter- and intra-molecular basis set superposition error in Hartree-Fock and density functional theory calculations for large systems. Journal of Chemical Physics, 2012, 136, 154101. | 1.2 | 556 |
| 5982 | JACOB: A Dynamic Database for Computational Chemistry Benchmarking. Journal of Chemical Information and Modeling, 2012, 52, 3255-3262. | 2.5 | 4 |
| 5983 | Absorption spectra of natural pigments as sensitizers in solar cells by TD-DFT and MRPT2: protonated cyanidin. Physical Chemistry Chemical Physics, 2012, 14, 16130. | 1.3 | 10 |
| 5984 | Can the Closed-Shell DFT Methods Describe the Thermolysis of 1,2-Dioxetanone?. Journal of Chemical Theory and Computation, 2012, 8, 4359-4363. | 2.3 | 31 |
| 5985 | High pressure ices. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 745-750. | 3.3 | 92 |
| 5986 | Carbenoid Alkene Insertion Reactions of Oxiranyllithiums. Journal of Organic Chemistry, 2012, 77, 8605-8614. | 1.7 | 7 |
| 5987 | Polyoxopalladates Encapsulating 8-Coordinated Metal Ions, [MO ₈ Pd ^{II}] ₁₂ L ₈]·nH ₂ O (M = Tl, Pb, Bi, Sb, As, Sn, Te, Se, Mo, W, V, Nb, Ta, Ti, Zr, Hf, U, Th, Pa, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr) ETQq0 0 0 rgBT /Overlock 10 Tf 50 | 1.9 | 58 |
| 5988 | 13214-13228. Dihydrogen Catalysis: A Degradation Mechanism for N ₂ -Fixation Intermediates. Journal of Physical Chemistry A, 2012, 116, 11618-11642. | 1.1 | 16 |
| 5989 | Ab Initio Calculations of the Interaction between CO ₂ and the Acetate Ion. Journal of Physical Chemistry A, 2012, 116, 11643-11650. | 1.1 | 50 |
| 5990 | Mechanism of H ₂ O ₂ Decomposition on Transition Metal Oxide Surfaces. Journal of Physical Chemistry C, 2012, 116, 9533-9543. | 1.5 | 223 |
| 5991 | TD-DFT Assessment of Functionals for Optical $\pi \rightarrow \pi^*$ Transitions in Solvated Dyes. Journal of Chemical Theory and Computation, 2012, 8, 2359-2372. | 2.3 | 403 |
| 5992 | The Reaction Mechanism of the Enantioselective Tsuji Allylation: Inner-Sphere and Outer-Sphere Pathways, Internal Rearrangements, and Asymmetric C-C Bond Formation. Journal of the American Chemical Society, 2012, 134, 19050-19060. | 6.6 | 103 |
| 5993 | Theoretical and experimental exploration of the photochemistry of resveratrol: beyond the simple double bond isomerization. Organic and Biomolecular Chemistry, 2012, 10, 9175. | 1.5 | 37 |
| 5994 | Cytochrome P450-Catalyzed Degradation of Nicotine: Fundamental Parameters Determining Hydroxylation by Cytochrome P450 2A6 at the β -Carbon or the α -Methyl Carbon. Journal of Physical Chemistry B, 2012, 116, 7827-7840. | 1.2 | 14 |
| 5995 | Performance of dispersion-corrected density functional theory for the interactions in ionic liquids. Physical Chemistry Chemical Physics, 2012, 14, 4875. | 1.3 | 202 |
| 5996 | Theoretical assessment of the viability of thermal [2+2] processes for formation of plumisclerin A. Tetrahedron Letters, 2012, 53, 6919-6922. | 0.7 | 12 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 5997 | Concise Total Synthesis and Stereochemical Analysis of Tetraponerines T3 and T4. <i>Journal of Organic Chemistry</i> , 2012, 77, 10340-10346. | 1.7 | 41 |
| 5998 | A Homologous Series of First-Row Transition-Metal Complexes of 2,2'-Bipyridine and their Ligand Radical Derivatives: Trends in Structure, Magnetism, and Bonding. <i>Inorganic Chemistry</i> , 2012, 51, 12301-12312. | 1.9 | 49 |
| 5999 | Palladacyclic Imidazoline-Naphthalene Complexes: Synthesis and Catalytic Performance in Pd(II)-Catalyzed Enantioselective Reactions of Allylic Trichloroacetimidates. <i>Journal of Organic Chemistry</i> , 2012, 77, 1939-1951. | 1.7 | 25 |
| 6000 | Selective Formation of 1,4-Disubstituted Triazoles from Ruthenium-Catalyzed Cycloaddition of Terminal Alkynes and Organic Azides: Scope and Reaction Mechanism. <i>Organometallics</i> , 2012, 31, 4904-4915. | 1.1 | 47 |
| 6001 | Atropisomers of Hindered Triarylisocyanurates: Structure, Conformation, Stereodynamics, and Absolute Configuration. <i>Journal of Organic Chemistry</i> , 2012, 77, 3373-3380. | 1.7 | 13 |
| 6002 | Chelation-Controlled Addition of Organozincs to α -Chloro Aldimines. <i>Journal of the American Chemical Society</i> , 2012, 134, 17599-17604. | 6.6 | 30 |
| 6003 | Energetic Study Applied to the Knowledge of the Structural and Electronic Properties of Monofluorobenzonitriles. <i>Journal of Organic Chemistry</i> , 2012, 77, 4312-4322. | 1.7 | 18 |
| 6004 | Retaining Glycosyltransferase Mechanism Studied by QM/MM Methods: Lipopolysaccharyl- β -1,4-galactosyltransferase C Transfers β -Galactose via an Oxocarbenium Ion-like Transition State. <i>Journal of the American Chemical Society</i> , 2012, 134, 4743-4752. | 6.6 | 89 |
| 6005 | Phase transition study of confined water molecules inside carbon nanotubes: Hierarchical multiscale method from molecular dynamics simulation to ab initio calculation. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 38, 40-49. | 1.3 | 11 |
| 6006 | Performance of Effective Core Potentials for Density Functional Calculations on 3d Transition Metals. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 80-90. | 2.3 | 58 |
| 6007 | Nitro-Substituted 4-[(Phenylmethylene)imino]phenolates: Solvatochromism and Their Use as Solvatochromic Switches and as Probes for the Investigation of Preferential Solvation in Solvent Mixtures. <i>Journal of Organic Chemistry</i> , 2012, 77, 10668-10679. | 1.7 | 52 |
| 6008 | The mechanism of the amine-catalysed isomerization of dialkyl maleate: a computational study. <i>Molecular Physics</i> , 2012, 110, 467-482. | 0.8 | 5 |
| 6009 | An Efficient One-Pot Three-Component Synthesis of Highly Functionalized Coumarin Fused Indenodihydropyridine and Chromeno[4,3-b]quinoline Derivatives. <i>Heterocycles</i> , 2012, 85, 1629. | 0.4 | 15 |
| 6010 | DFT Studies on Copper-Catalyzed Arylation of Aromatic C-H Bonds. <i>Organometallics</i> , 2012, 31, 560-569. | 1.1 | 50 |
| 6011 | ¹⁵ N NMR Studies of tautomerism. <i>International Reviews in Physical Chemistry</i> , 2012, 31, 567-629. | 0.9 | 25 |
| 6012 | Methane Dehydrogenation and Coupling to Ethylene over a Mo/HZSM-5 Catalyst: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 4060-4070. | 1.5 | 39 |
| 6013 | Can Metallapyrimidines Be Aromatic? A Computational Study into a New Class of Metallacycles. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4950-4959. | 2.3 | 20 |
| 6014 | Performance of Gradient-Corrected and Hybrid Density Functional Theory: Role of the Underlying Local Density Approximation and the Gradient Correction. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4899-4906. | 2.3 | 16 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6015 | Model Iron ^{II} Oxo Species and the Oxidation of Imidazole: Insights into the Mechanism of OvoA and EgtB?. <i>Inorganic Chemistry</i> , 2012, 51, 13351-13356. | 1.9 | 36 |
| 6016 | M11-L: A Local Density Functional That Provides Improved Accuracy for Electronic Structure Calculations in Chemistry and Physics. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 117-124. | 2.1 | 531 |
| 6017 | A Phosphorescent C ¹ S ² Cyclometalated Platinum(II) Dibenzothiophene NHC Complex. <i>Organometallics</i> , 2012, 31, 7447-7452. | 1.1 | 58 |
| 6018 | Synthesis and Characterization of Novel Iron(II) Complexes with Tetradentate Bis(N-heterocyclic) Tj ETQq1 1 0.784314 rgBT /Overlock | 1.1 | 64 |
| 6019 | Two-Component Relativistic Calculations of Electric-Field Gradients Using Exact Decoupling Methods: Spin ^{II} orbit and Picture-Change Effects. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4239-4248. | 2.3 | 62 |
| 6020 | Hybrid Quantum and Classical Simulations of the Formate Dehydrogenase Catalyzed Hydride Transfer Reaction on an Accurate Semiempirical Potential Energy Surface. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4786-4796. | 2.3 | 25 |
| 6021 | A Novel Metal Organic Compound of Al(III): Synthesis, Crystal Structure, Spectroscopic and Theoretical Study. <i>Journal of Chemical Crystallography</i> , 2012, 42, 1152-1161. | 0.5 | 3 |
| 6022 | Organocatalytic enantioselective pyrazol-3-one addition to maleimides: Reactivity and stereochemical course. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 1645. | 1.5 | 60 |
| 6023 | Rotational barriers of biphenyls having heavy heteroatoms as ortho-substituents: experimental and theoretical determination of steric effects. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 1847. | 1.5 | 53 |
| 6024 | Prediction of Structure and Properties of Boron-Based Covalent Organic Frameworks by a First-Principles Derived Force Field. <i>Journal of Physical Chemistry C</i> , 2012, 116, 4921-4929. | 1.5 | 52 |
| 6025 | Hybrid functionals and <i>G</i> / <i>W</i> approximation in the FLAPW method. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 293201. | 0.7 | 33 |
| 6026 | First evidence for the formation of technetium oxosulfide complexes: synthesis, structure and characterization. <i>Dalton Transactions</i> , 2012, 41, 6291. | 1.6 | 12 |
| 6027 | Can density functional theory describe the NO(X ²)-Ar and NO(A ² Σ ⁺)-Ar van der Waals complexes?. <i>Journal of Chemical Physics</i> , 2012, 136, 244313. | 1.2 | 15 |
| 6028 | Theoretical study of structural and optical properties of noble metal cluster ^{II} dipeptide hybrids at defect centers of MgO. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 9330. | 1.3 | 5 |
| 6029 | Vibrational Spectra of Phosphate Ions in Aqueous Solution Probed by First-Principles Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2466-2474. | 1.1 | 41 |
| 6030 | Unrestricted Prescriptions for Open-Shell Singlet Diradicals: Using Economical Ab Initio and Density Functional Theory to Calculate Singlet ^{II} Triplet Gaps and Bond Dissociation Curves. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4922-4929. | 1.1 | 42 |
| 6031 | Structure and Redox Behavior of Iron Oxophlorin and Role of Electron Transfer in the Heme Degradation Process. <i>Inorganic Chemistry</i> , 2012, 51, 12857-12866. | 1.9 | 3 |
| 6032 | Theoretical study of Au ⁿ -CO, n = 1 ^{II} 14: The dopant vanadium enhances CO adsorption on gold clusters. <i>Journal of Chemical Physics</i> , 2012, 137, 164312. | 1.2 | 26 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6033 | Changes in Charge Distribution, Molecular Volume, Accessible Surface Area and Electronic Structure along the Reaction Coordinate for a Carbocationic Triple Shift Rearrangement of Relevance to Diterpene Biosynthesis. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8902-8909. | 1.1 | 21 |
| 6034 | Palladium(II)-Catalyzed Enantioselective Synthesis of 2-Vinyl Oxygen Heterocycles. <i>Journal of Organic Chemistry</i> , 2012, 77, 1961-1973. | 1.7 | 60 |
| 6035 | Investigating the Calculation of Anharmonic Vibrational Frequencies Using Force Fields Derived from Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4417-4425. | 1.1 | 42 |
| 6036 | Efficient Förster Resonance Energy Transfer in 1,2,3-Triazole Linked BODIPY-Zn(II) Meso-tetraphenylporphyrin Donor-Acceptor Arrays. <i>Inorganic Chemistry</i> , 2012, 51, 13114-13122. | 1.9 | 60 |
| 6037 | Rearrangement of Tridentate [OSO]-Type Ligands and Migratory Insertion Reaction Mechanisms in Cyclopentadienyl Tantalum Complexes. <i>Organometallics</i> , 2012, 31, 7052-7062. | 1.1 | 8 |
| 6038 | The R ₃ O ⁺ ·H Hydrogen Bond: Toward a Tetracoordinate Oxadionium(2+) Ion. <i>Journal of the American Chemical Society</i> , 2012, 134, 707-714. | 6.6 | 39 |
| 6039 | A comparison of two-component and four-component approaches for calculations of spin-spin coupling constants and NMR shielding constants of transition metal cyanides. <i>Journal of Chemical Physics</i> , 2012, 137, 014311. | 1.2 | 34 |
| 6040 | Novel cinnamic acid/4-aminoquinoline conjugates bearing non-proteinogenic amino acids: Towards the development of potential dual action antimalarials. <i>European Journal of Medicinal Chemistry</i> , 2012, 54, 887-899. | 2.6 | 50 |
| 6041 | Derivation and Systematic Validation of a Refined All-Atom Force Field for Phosphatidylcholine Lipids. <i>Journal of Physical Chemistry B</i> , 2012, 116, 3164-3179. | 1.2 | 486 |
| 6042 | Cobalt analogues of Roussin's red salt esters: a density functional study. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12332. | 1.3 | 1 |
| 6043 | Prognostication of the anticorrosive activity in the series of pentenylarylamines and their industrial introduction. <i>Russian Journal of Applied Chemistry</i> , 2012, 85, 1182-1185. | 0.1 | 0 |
| 6044 | Evaluation of some phenothiazine derivatives as corrosion inhibitors for bronze in weakly acidic solution. <i>Corrosion Science</i> , 2012, 63, 275-286. | 3.0 | 53 |
| 6045 | Coordination Effects on Electron Distributions for Rhodium Complexes of the Redox-Active Bis(3,5-di-tert-butyl-2-phenolate)amide Ligand. <i>Inorganic Chemistry</i> , 2012, 51, 12606-12618. | 1.9 | 30 |
| 6046 | New Insights into the Electronic Structure and Reactivity of One-Electron Oxidized Copper(II)-(Disalicylidene)diamine Complexes. <i>Inorganic Chemistry</i> , 2012, 51, 12450-12461. | 1.9 | 71 |
| 6047 | Violation of a local form of the Lieb-Oxford bound. <i>Physical Review A</i> , 2012, 85, . | 1.0 | 12 |
| 6048 | Theoretical Elucidation of the Mechanism of Cleavage of the Aromatic C-Cl Bond in Quinoxaline by a Tungsten-Based Complex [W(PMe ₃) ₄ (i-Pr) ₂ CH ₂ PMe ₂)]H. <i>Chemistry - A European Journal</i> , 2012, 18, 15537-15545. | 1.7 | 7 |
| 6049 | Re-examining the Mechanisms of Competing Pericyclic Reactions of 1,3,7-Octatriene. <i>Chemistry - A European Journal</i> , 2012, 18, 11029-11035. | 1.7 | 6 |
| 6050 | Solid-State ⁷³ Ge...NMR Spectroscopy of Simple Organogermanes. <i>Chemistry - A European Journal</i> , 2012, 18, 13770-13779. | 1.7 | 13 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6051 | Reversible Binding of Molecular Oxygen to Catecholate and Amidophenolate Complexes of Sb ^V : Electronic and Steric Factors. <i>ChemPhysChem</i> , 2012, 13, 3773-3776. | 1.0 | 40 |
| 6052 | Etching Silicon with HF/HNO ₃ /H ₂ SO ₄ /H ₂ O Mixtures: Unprecedented Formation of Trifluorosilane, Hexafluorodisiloxane, and Si-F Surface Groups. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 5714-5721. | 1.0 | 27 |
| 6053 | Facile Oxidative Rearrangements Using Hypervalent Iodine Reagents. <i>ChemistryOpen</i> , 2012, 1, 245-250. | 0.9 | 66 |
| 6054 | Induced chirality in fisetin upon binding to serum albumin: experimental circular dichroism and TDDFT calculations. <i>Journal of Molecular Modeling</i> , 2012, 18, 4381-4387. | 0.8 | 9 |
| 6055 | Quantum chemical modeling of UV Spectra of Polyurethane Structural Fragments. <i>Journal of Applied Spectroscopy</i> , 2012, 79, 339-343. | 0.3 | 1 |
| 6056 | Assignments and forms of stretching vibrations of 1,4-naphthoquinone carbonyl groups. <i>Journal of Applied Spectroscopy</i> , 2012, 79, 675-686. | 0.3 | 3 |
| 6057 | Molecular Simulations of Polyphosphazenes for Biomedical Applications. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2012, 22, 973-984. | 1.9 | 21 |
| 6058 | Bipolarons and polaron pairs in oligopyrrole dications. <i>Computational and Theoretical Chemistry</i> , 2012, 993, 7-12. | 1.1 | 9 |
| 6059 | Correlating ETD fragment ion intensities with peptide ion conformational and electronic structure. <i>International Journal of Mass Spectrometry</i> , 2012, 330-332, 207-219. | 0.7 | 11 |
| 6060 | Mechanistic insights into the hydrosilylation of allyl compounds: Evidence for different coexisting reaction pathways. <i>Journal of Catalysis</i> , 2012, 295, 1-14. | 3.1 | 30 |
| 6061 | Reactions of Group 3 Metals with OF ₂ : Infrared Spectroscopic and Theoretical Investigations of the Group 3 Oxydifluoride OMF ₂ and Oxyfluoride OMF Molecules. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10115-10121. | 1.1 | 10 |
| 6062 | Which oxidation state is preferable at S0 state in oxygen-evolving complex, Mn ₄ (II, III, IV, IV) or Mn ₄ (III, IV). <i>J. Phys. Chem. B</i> , 2012, 116, 10115-10121. | 1.2 | 9 |
| 6063 | Reduction Pathways of 2,4,6-Trinitrotoluene: An Electrochemical and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 4243-4251. | 1.5 | 88 |
| 6064 | Superacid-Promoted Ionization of Alkanes Without Carbonium Ion Formation: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9979-9984. | 1.1 | 14 |
| 6065 | Molecular Redox: Revisiting the Electronic Structures of the Group 9 Metallocorroles. <i>Inorganic Chemistry</i> , 2012, 51, 12473-12482. | 1.9 | 17 |
| 6066 | Tuning the optical properties of dithienylethenes: Theoretical insights. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2012, 247, 30-41. | 2.0 | 29 |
| 6067 | Thermodynamic Study on the Complexation of Am(III) and Eu(III) with Tetradentate Nitrogen Ligands: A Probe of Complex Species and Reactions in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2012, 116, 504-511. | 1.1 | 46 |
| 6068 | DFT study of metal-complex structural variation on tensile force profiles. <i>Chemical Physics Letters</i> , 2012, 554, 96-101. | 1.2 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6069 | Dipole moment and polarizability of the low-lying excited states of uracil. <i>Chemical Physics Letters</i> , 2012, 546, 24-29. | 1.2 | 25 |
| 6070 | Aniline-1,4-benzoquinone as a model system for the characterization of products from aniline oligomerization in low acidic media. <i>Chemical Physics Letters</i> , 2012, 551, 130-133. | 1.2 | 34 |
| 6071 | Enhanced Raman spectrum of pyrazine with the aid of resonant electron dynamics in a nearby cluster. <i>Chemical Physics Letters</i> , 2012, 550, 52-57. | 1.2 | 4 |
| 6072 | Ligand exchange processes on solvated beryllium cations VII – water exchange on cationic $[\text{Be}(\text{H}_2\text{O})_3(\text{Ln})]^{2+n}$ (Ln: 4-O-Py ⁺ , Py, 4-(Py)-Py ⁺ , 3,5-(Py) ₂ -Py ²⁺ , 3,4,5-(Py) ₃ -Py ³⁺). <i>RSC Advances</i> , 2012, 2, 5815. | 1.7 | 5 |
| 6073 | On the electronic structure and conflicting d-orbital aromaticity in the Re_3O_3^+ cluster. <i>RSC Advances</i> , 2012, 2, 2707. | 1.7 | 16 |
| 6074 | Synthesis, Cu(II) complexation, Cu-labeling and biological evaluation of cross-bridged cyclam chelators with phosphonate pendant arms. <i>Dalton Transactions</i> , 2012, 41, 1938-1950. | 1.6 | 95 |
| 6075 | Quantitative integral cross sections for the $\text{H} + \text{CO}_2 \rightarrow \text{OH} + \text{CO}$ reaction from a density functional theory-based potential energy surface. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 16699. | 1.3 | 9 |
| 6076 | Crystal structure, electronic properties and cytotoxic activity of palladium chloride complexes with monosubstituted pyridines. <i>Dalton Transactions</i> , 2012, 41, 658-666. | 1.6 | 30 |
| 6077 | Silver cluster-biomolecule hybrids: from basics towards sensors. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 9282. | 1.3 | 51 |
| 6078 | Mechanistic identification and improvement of a direct enantioconvergent transformation in copper-catalyzed asymmetric allylic alkylation. <i>Chemical Science</i> , 2012, 3, 1062-1069. | 3.7 | 47 |
| 6079 | Probing differences in binding of methylbenzylamine enantiomers to chiral cobalt(II) salen complexes. <i>Dalton Transactions</i> , 2012, 41, 6861. | 1.6 | 3 |
| 6080 | Spectroscopic and magnetic properties of an iodo CoI tripod phosphine complex. <i>Dalton Transactions</i> , 2012, 41, 11788. | 1.6 | 6 |
| 6081 | Photoreaction channels of the guanine-cytosine base pair explored by long-range corrected TDDFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8866. | 1.3 | 32 |
| 6082 | Different coordination modes of 2-(diphenylphosphino)azobenzenes in complexation with hard and soft metals. <i>Dalton Transactions</i> , 2012, 41, 11491. | 1.6 | 7 |
| 6083 | Electronic Ground-State and Orbital Ordering of Iron Phthalocyanine on H/Si(111) Unraveled by Spatially Resolved Tunneling Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2012, 116, 20882-20886. | 1.5 | 24 |
| 6084 | Development, Implementation, and Application of an Analytic Second Derivative Formalism for the Normalized Elimination of the Small Component Method. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2617-2629. | 2.3 | 44 |
| 6085 | Charge-Transfer Excitations in Uranyl Tetrachloride ($[\text{UO}_2\text{Cl}_4]^{2-}$): How Reliable are Electronic Spectra from Relativistic Time-Dependent Density Functional Theory?. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7397-7404. | 1.1 | 47 |
| 6086 | Apparent or real water exchange reactions on $[\text{Zn}(\text{H}_2\text{O})_4(\text{L})]^{2+} \cdot 2\text{H}_2\text{O}$ (L = sp-nitrogen donor ligands)? A quantum chemical investigation. <i>Dalton Transactions</i> , 2012, 41, 6932. | 1.6 | 8 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6087 | The structure of 5-cyanoindole in the ground and the lowest electronically excited singlet states, deduced from rotationally resolved electronic spectroscopy and ab initio theory. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10266. | 1.3 | 34 |
| 6088 | The neutral analogue of Roussin's red salt anion: a density functional study. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 5998. | 1.3 | 2 |
| 6089 | Unusually Fast 1,6-H Shifts of Enolic Hydrogens in Peroxy Radicals: Formation of the First-Generation C ₂ and C ₃ Carbonyls in the Oxidation of Isoprene. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6134-6141. | 1.1 | 34 |
| 6090 | Oxidation Mechanism of Methionine by HO [•] Radical: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5349-5354. | 1.2 | 9 |
| 6091 | Photoinitiators with $\hat{\text{I}}^2$ -Phenyllogous Cleavage: An Evaluation of Reaction Mechanisms and Performance. <i>Macromolecules</i> , 2012, 45, 1737-1745. | 2.2 | 18 |
| 6092 | Critical appraisal of excited state nonadiabatic dynamics simulations of 9 <i>H</i> -adenine. <i>Journal of Chemical Physics</i> , 2012, 137, 22A503. | 1.2 | 102 |
| 6093 | Experimental and theoretical study of the degradation of malonamide extractant molecules under ionizing radiation. <i>RSC Advances</i> , 2012, 2, 3954. | 1.7 | 6 |
| 6094 | Cyclic bis($\hat{\text{I}}^2$ -diketonate)- and bis($\hat{\text{I}}^2$ -ketoesterate)-bridged titanium and zirconium alkoxide derivatives. <i>Dalton Transactions</i> , 2012, 41, 2346-2353. | 1.6 | 17 |
| 6095 | Fusing cubanes to 1,5-hexadiene. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14756. | 1.3 | 0 |
| 6096 | Aza-boron-dipyrromethene dyes: TD-DFT benchmarks, spectral analysis and design of original near-IR structures. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 157-164. | 1.3 | 100 |
| 6097 | Fully relativistic coupled cluster and DFT study of electric field gradients at Hg in 199Hg compounds. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 2651. | 1.3 | 31 |
| 6098 | Method/basis set dependence of NICS values among metallic nano-clusters and hydrocarbons. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 3471. | 1.3 | 16 |
| 6099 | A new structural model for disorder in vaterite from first-principles calculations. <i>CrystEngComm</i> , 2012, 14, 44-47. | 1.3 | 71 |
| 6100 | Confusion of Möbius aromaticity: disruption of annulenic pathway in singly N-confused [28]hexaphyrin and its mono-Pd(II) complex. <i>Dalton Transactions</i> , 2012, 41, 6283. | 1.6 | 18 |
| 6101 | The interaction of His337 with the Mn4Ca cluster of photosystem II. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 4651. | 1.3 | 32 |
| 6102 | Activation of C [•] Cl by ground-state aluminum atoms: an EPR and DFT investigation. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 367-374. | 1.3 | 5 |
| 6103 | A theoretical study on the stereoconvergency of the intramolecular radical cation [2+2] cycloadditions of bis(styrenes). <i>RSC Advances</i> , 2012, 2, 9932. | 1.7 | 6 |
| 6104 | Rhenium complexes of peripherally $\hat{\text{I}}^2$ -extended N-confused porphyrins. <i>Chemical Science</i> , 2012, 3, 3241. | 3.7 | 24 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6105 | A density functional study of the relative stability of intermediates in a McMurry coupling reaction. <i>Journal of Coordination Chemistry</i> , 2012, 65, 1484-1492. | 0.8 | 2 |
| 6106 | Theoretical Insight into PtCl ₂ -Catalyzed Isomerization of Cyclopropenes to Allenes. <i>Organometallics</i> , 2012, 31, 4769-4778. | 1.1 | 13 |
| 6107 | Electron Paramagnetic Resonance Spectroscopic Evidence for the Interaction of HAlOH with Water Molecules. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4267-4273. | 1.1 | 10 |
| 6108 | Intramolecular Electronic Couplings in Class II/III Organic Mixed-Valence Systems of Bis(1,4-dimethoxybenzene). <i>Journal of Physical Chemistry B</i> , 2012, 116, 14126-14135. | 1.2 | 14 |
| 6109 | Carbon-Oxygen Bond Formation via Organometallic Baeyer-Villiger Transformations: A Computational Study on the Impact of Metal Identity. <i>Journal of the American Chemical Society</i> , 2012, 134, 2332-2339. | 6.6 | 44 |
| 6110 | Kinetic and Mechanistic Studies of Base-Catalyzed Phenylselenoetherification of <i>Z</i> - and <i>E</i> -Hex-4-en-1-ols. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7783-7790. | 1.1 | 10 |
| 6111 | Role of Inter- and Intramolecular Bonding on Impact Sensitivity. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11008-11014. | 1.1 | 9 |
| 6112 | Application of Screened Hybrid Density Functional Theory to Ammonia Decomposition on Silicon. <i>Journal of Physical Chemistry C</i> , 2012, 116, 26396-26404. | 1.5 | 17 |
| 6113 | SCC-DFTB Parametrization for Boron and Boranes. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1153-1163. | 2.3 | 26 |
| 6114 | Solvatochromic shifts of polar and non-polar molecules in ambient and supercritical water: A sequential quantum mechanics/molecular mechanics study including solute-solvent electron exchange-correlation. <i>Journal of Chemical Physics</i> , 2012, 137, 214504. | 1.2 | 16 |
| 6115 | Magnetic Mn and Co Complexes with a Large Polycyclic Aromatic Substituted Nitronyl Nitroxide. <i>Inorganic Chemistry</i> , 2012, 51, 3138-3145. | 1.9 | 38 |
| 6116 | Vibrational and Electronic Circular Dichroism of Dimethyl Mesobilirubins-XIII±. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5628-5636. | 1.2 | 11 |
| 6117 | Multilevel X-Pol: A Fragment-Based Method with Mixed Quantum Mechanical Representations of Different Fragments. <i>Journal of Physical Chemistry B</i> , 2012, 116, 6781-6788. | 1.2 | 32 |
| 6118 | Do 12-Membered Cycloalkane Rings Only Exist As One Conformation in the Solid-State? A Detailed Solid-State Analysis Involving Polymorphs of N,N'-Biscyclododecyl Pyromellitic Diimide. <i>Crystal Growth and Design</i> , 2012, 12, 5908-5916. | 1.4 | 6 |
| 6119 | Theoretical Insight into the Mechanism of CO Inserting into the N-H Bond of the Iron(II) Amido Complex (dmpe) ₂ Fe(H)(NH ₂): An Unusual Self-Promoted Reaction. <i>Organometallics</i> , 2012, 31, 365-371. | 1.1 | 5 |
| 6120 | OMS, OM(Ĥ ² -SO), and OM(Ĥ ² -SO)(Ĥ ² -SO) ₂ Molecules (M = Tj ETQq1 1 0.784314 7415-7424. | 1.9 | 25 |
| 6121 | Synthesis of Alkenyl Ylide Complexes from Reactions of ReOCl ₂ (OEt)(PPh ₃) ₂ with Alkynols. <i>Organometallics</i> , 2012, 31, 7085-7092. | 1.1 | 11 |
| 6122 | Role of Ĥ-Acceptor Effects in Controlling the Lability of Novel Monofunctional Pt(II) and Pd(II) Complexes: Crystal Structure of [Pt(triipyridinedimethane)Cl]Cl. <i>Inorganic Chemistry</i> , 2012, 51, 1516-1529. | 1.9 | 48 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6123 | Gas-Phase Chemical Dynamics Simulations on the Bifurcating Pathway of the Pimaradienyl Cation Rearrangement: Role of Enzymatic Steering in Abietic Acid Biosynthesis. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1212-1222. | 2.3 | 46 |
| 6124 | Influence of the Alkyl Substituents Spacing on the Solar Cell Performance of Benzodithiophene Semiconducting Polymers. <i>Macromolecules</i> , 2012, 45, 772-780. | 2.2 | 26 |
| 6126 | Ab Initio Study of the Emissive Charge-Transfer States of Solvated Chromophore-Functionalized Silsesquioxanes. <i>Journal of the American Chemical Society</i> , 2012, 134, 6944-6947. | 6.6 | 72 |
| 6127 | Revisit of 4,4'-Diaminodiphenyl Sulfone Photophysics in Different Solvents. <i>Industrial & Engineering Chemistry Research</i> , 2012, 51, 2505-2514. | 1.8 | 19 |
| 6128 | Assessment of Density Functional Theory in Predicting Structures and Free Energies of Reaction of Atmospheric Prenucleation Clusters. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2071-2077. | 2.3 | 168 |
| 6129 | Structure-Guided Topographic Mapping and Mutagenesis to Elucidate Binding Sites for the Human Ether-a-Go-Go-Related Gene 1 Potassium Channel (KCNH2) Activator NS1643. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2012, 342, 441-452. | 1.3 | 29 |
| 6130 | DFT and TD-DFT study on the electronic structures and phosphorescent properties of 6-phenyl-2,2'-bipyridine tridentate iridium(III) complexes and their isomer. <i>Dalton Transactions</i> , 2012, 41, 8441. | 1.6 | 34 |
| 6131 | Stability and Spectroscopic Properties of Singly and Doubly Charged Anions. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5604-5617. | 1.1 | 14 |
| 6132 | Fully Relativistic Calculations of Faraday and Nuclear Spin-Induced Optical Rotation in Xenon. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 91-98. | 2.3 | 23 |
| 6133 | Modification of Lipid Bilayer Structure by Diacylglycerol: A Comparative Study of Diacylglycerol and Cholesterol. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 749-758. | 2.3 | 41 |
| 6134 | Low-Energy States of Manganese(II) Oxo Corrole and Corrolazine: Multiconfiguration Reference ab Initio Calculations. <i>Inorganic Chemistry</i> , 2012, 51, 4002-4006. | 1.9 | 37 |
| 6135 | Phase Behavior and Conductivity of Sulfonated Block Copolymers Containing Heterocyclic Diazole-Based Ionic Liquids. <i>Macromolecules</i> , 2012, 45, 8702-8713. | 2.2 | 46 |
| 6136 | Ab Initio Calculation of the Electronic Absorption of Functionalized Octahedral Silsesquioxanes via Time-Dependent Density Functional Theory with Range-Separated Hybrid Functionals. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1137-1145. | 1.1 | 52 |
| 6137 | Electronic Absorption Spectra from MM and <i>ab Initio</i> QM/MM Molecular Dynamics: Environmental Effects on the Absorption Spectrum of Photoactive Yellow Protein. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 5092-5106. | 2.3 | 158 |
| 6138 | Theoretical Investigations on Charge-Transfer Properties of Novel High Mobility n-Channel Organic Semiconductors - Diazapentacene Derivatives. <i>Journal of Physical Chemistry C</i> , 2012, 116, 22749-22758. | 1.5 | 28 |
| 6139 | Activation of C=O and C=C Bonds and Formation of Novel HAlOH-Ether Complexes: An EPR Study of the Reaction of Ground-State Al Atoms with Methyl ethyl Ether and Diethyl Ether. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2439-2452. | 1.1 | 6 |
| 6140 | Iridium-Catalyzed [2 + 2 + 2] Cycloaddition of β,γ -Diynes with Nitriles. <i>Journal of the American Chemical Society</i> , 2012, 134, 10515-10531. | 6.6 | 120 |
| 6141 | M=O Bond-Stretching Energy Landscapes for M_2 (dimen) $_4$ ²⁺ (M = Ti, Zr, Hf, Th, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr). <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1051-1061. | 1.9 | 16 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6142 | Implications of Binding Mode and Active Site Flexibility for Inhibitor Potency against the Salicylate Synthase from <i>Mycobacterium tuberculosis</i> . <i>Biochemistry</i> , 2012, 51, 4868-4879. | 1.2 | 31 |
| 6143 | Reliability of Approximate Methods to Study Tip-Functionalized Single-Wall Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25401-25406. | 1.5 | 12 |
| 6144 | UV-Induced Unimolecular Photochemistry of Diketene Isolated in Cryogenic Inert Matrices. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2131-2140. | 1.1 | 16 |
| 6145 | Cp* Iridium Precatalysts for Selective C-H Oxidation via Direct Oxygen Insertion: A Joint Experimental/Computational Study. <i>ACS Catalysis</i> , 2012, 2, 208-218. | 5.5 | 82 |
| 6146 | Franck-Condon Dominates the Surface-Enhanced Raman Scattering of 3-Methylpyridine: Propensity Rules of the Charge-Transfer Mechanism under Reduced Symmetry. <i>Journal of Physical Chemistry C</i> , 2012, 116, 23639-23645. | 1.5 | 39 |
| 6147 | Unusual Low-Vibrational C=O Mode of COOH Can Distinguish between Carboxylated Zigzag and Armchair Single-Wall Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 26072-26083. | 1.5 | 13 |
| 6148 | Intersubunit Electron Transfer (IET) in Quantum Dots/Graphene Complex: What Features Does IET Endow the Complex with?. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15833-15838. | 1.5 | 28 |
| 6149 | Electronic Excitations in Epicocconone Analogues: TDDFT Methodological Assessment Guided by Experiment. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8634-8643. | 1.1 | 19 |
| 6150 | Mechanistic Insights into the Aerobic Copper(I)-Catalyzed Cross-Coupling of S-Acyl Thiosalicylamide Thiol Esters and Boronic Acids. <i>Organometallics</i> , 2012, 31, 7958-7968. | 1.1 | 14 |
| 6151 | Theoretical Study of the O ₂ + Al ₄ (Tetrahedral) System in Its Singlet State and Comparisons with Its Triplet State. <i>Journal of Physical Chemistry C</i> , 2012, 116, 16430-16435. | 1.5 | 5 |
| 6152 | Pulse Q-Band EPR and ENDOR Spectroscopies of the Photochemically Generated Monoprotonated Benzosemiquinone Radical in Frozen Alcoholic Solution. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8890-8900. | 1.2 | 9 |
| 6153 | Folding-Reaction Coupling in a Self-Cleaving Protein. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3871-3879. | 2.3 | 12 |
| 6154 | Theoretical-Experimental Study of Formic Acid Photofragmentation in the Valence Region. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6693-6701. | 1.1 | 7 |
| 6155 | Carbon Monoxide, Isocyanide, and Nitrile Complexes of Cationic, d ⁰ Vanadium Bisimides: π -Back Bonding Derived from the π Symmetry, Bonding Metal Bisimido Ligand Orbitals. <i>Inorganic Chemistry</i> , 2012, 51, 13334-13344. | 1.9 | 35 |
| 6156 | Parallel Implementation of Multireference Coupled-Cluster Theories Based on the Reference-Level Parallelism. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 487-497. | 2.3 | 25 |
| 6157 | Why Nature Eschews the Concerted [2 + 2 + 2] Cycloaddition of a Nonconjugated Cyanodiene. Computational Study of a Pyridine Synthesis Involving an Ene-Diels-Alder-Bimolecular Hydrogen-Transfer Mechanism. <i>Journal of Organic Chemistry</i> , 2012, 77, 1533-1538. | 1.7 | 24 |
| 6158 | New Insights into Frustrated Lewis Pairs: Structural Investigations of Intramolecular Phosphane-Borane Adducts by Using Modern Solid-State NMR Techniques and DFT Calculations. <i>Journal of the American Chemical Society</i> , 2012, 134, 4236-4249. | 6.6 | 78 |
| 6159 | Calculation and visualization of free energy barriers for several VOCs and TNT in HKUST-1. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 15438. | 1.3 | 13 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6160 | <i>trans</i> -[Fe(cyclam)(C ₂ R) ₂] ⁺ : A New Family of Iron(III) Bis-Alkynyl Compounds. <i>Organometallics</i> , 2012, 31, 6199-6206. | 1.1 | 34 |
| 6161 | Bottom-Up View of Water Network-Mediated CO ₂ Reduction Using Cryogenic Cluster Ion Spectroscopy and Direct Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2012, 116, 903-912. | 1.1 | 19 |
| 6162 | Computational Insights into Uranium Complexes Supported by Redox-Active $\hat{\pm}$ -Diimine Ligands. <i>Inorganic Chemistry</i> , 2012, 51, 2058-2064. | 1.9 | 25 |
| 6163 | Thermodynamics of Titanium and Vanadium Reduction in Non-Aqueous Environment Calculated at Various Levels of Theory. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1464-1468. | 1.1 | 3 |
| 6164 | Density Functional Investigation of the Water Oxidation by Iron Complexes Based on Tetradentate Nitrogen Ligands. <i>Inorganic Chemistry</i> , 2012, 51, 10850-10855. | 1.9 | 19 |
| 6165 | Combined Crossed Beam and Theoretical Studies of the N ₂ + C ₂ H ₄ Reaction and Implications for Atmospheric Models of Titan. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10467-10479. | 1.1 | 58 |
| 6166 | Cobalt-Centered Ten-Vertex Germanium Clusters: The Pentagonal Prism as an Alternative to Polyhedra Predicted by the Wade-Mingos Rules. <i>Inorganic Chemistry</i> , 2012, 51, 3498-3504. | 1.9 | 21 |
| 6167 | <i>cis</i> Influence in Models of Cobalt Corrins by DFT and TD-DFT Studies. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8836-8845. | 1.2 | 18 |
| 6168 | Energy Densities in the Strong-Interaction Limit of Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3097-3107. | 2.3 | 43 |
| 6169 | Unusual Isotope Effect in the Reaction of Chlorosilylene with Trimethylsilane- ¹³ C. Absolute Rate Studies and Quantum Chemical and Rice-Kassel-Marcus Calculations Provide Strong Evidence for the Involvement of an Intermediate Complex. <i>Journal of the American Chemical Society</i> , 2012, 134, 10493-10501. | 6.6 | 7 |
| 6170 | Theoretical Study of the Reductive Decomposition of Ethylene Sulfite: A Film-Forming Electrolyte Additive in Lithium Ion Batteries. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11025-11033. | 1.1 | 58 |
| 6171 | Glycerol Dehydration by the B ₁₂ -Independent Enzyme May Not Involve the Migration of a Hydroxyl Group: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 7076-7087. | 1.2 | 33 |
| 6172 | Experimental and Theoretical Charge Density Distribution in a Host-Guest System: Synthetic Terephthaloyl Receptor Complexed to Adipic Acid. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5618-5628. | 1.1 | 8 |
| 6173 | A Functional [NiFe]-Hydrogenase Model Compound That Undergoes Biologically Relevant Reversible Thiolate Protonation. <i>Journal of the American Chemical Society</i> , 2012, 134, 20745-20755. | 6.6 | 101 |
| 6174 | Self-Assembled Molecular Rafts at Liquid Liquid Interfaces for Four-Electron Oxygen Reduction. <i>Journal of the American Chemical Society</i> , 2012, 134, 498-506. | 6.6 | 87 |
| 6175 | Reactivity of Borylenes toward Ethyne, Ethene, and Methane. <i>Journal of the American Chemical Society</i> , 2012, 134, 17094-17103. | 6.6 | 27 |
| 6176 | Molecular Conformation in Organic Films from Quantum Chemistry ab Initio Calculations and Second Harmonic Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2012, 116, 26784-26790. | 1.5 | 5 |
| 6177 | Density functionals for surface science: Exchange-correlation model development with Bayesian error estimation. <i>Physical Review B</i> , 2012, 85, . | 1.1 | 1,087 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6178 | Obtaining Enhanced Circular Dichroism in [4]Heterohelicenic Analogues. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8744-8752. | 1.1 | 14 |
| 6179 | Isotope Effect in the Carbonyl Sulfide Reaction with O(³ P). <i>Journal of Physical Chemistry A</i> , 2012, 116, 3521-3526. | 1.1 | 20 |
| 6180 | Photoisomerization of <i>cis</i> -1-(3-Methyl-2-naphthyl)-2-phenylethene in Glassy Methylcyclohexane at 77 K. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5293-5298. | 1.1 | 6 |
| 6181 | Impact of Vibronic Couplings on Perceived Colors: Two Anthraquinones as a Working Example. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 468-471. | 2.1 | 82 |
| 6182 | Assessment of Theoretical Procedures for Calculating Barrier Heights for a Diverse Set of Water-Catalyzed Proton-Transfer Reactions. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4211-4221. | 1.1 | 92 |
| 6183 | Probing Electrospray Ionization Dynamics Using Differential Mobility Spectrometry: The Curious Case of 4-Aminobenzoic Acid. <i>Analytical Chemistry</i> , 2012, 84, 7857-7864. | 3.2 | 94 |
| 6184 | PERI-CC2: A Polarizable Embedded RI-CC2 Method. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3274-3283. | 2.3 | 75 |
| 6185 | Computed and Experimental Chemical Shift Parameters for Rigid and Flexible YAF Peptides in the Solid State. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1974-1983. | 1.2 | 30 |
| 6186 | Mode Recognition in UV Resonance Raman Spectra of Imidazole: Histidine Monitoring in Proteins. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9387-9395. | 1.2 | 15 |
| 6187 | Experimental and Theoretical Study of the Living Polymerization of <i>N</i> -Silylphosphoranimines. Synthesis of New Block Copolyphosphazenes. <i>Organometallics</i> , 2012, 31, 2571-2581. | 1.1 | 30 |
| 6188 | Infrared Multiple-Photon Dissociation Spectroscopy of Tripositive Ions: Lanthanum-Tryptophan Complexes. <i>Inorganic Chemistry</i> , 2012, 51, 4707-4710. | 1.9 | 12 |
| 6189 | Introducing the ELF Topological Analysis in the Field of Quasirelativistic Quantum Calculations. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2985-2990. | 2.3 | 43 |
| 6190 | Cyclic and Linear NiO ₂ : A Multireference Configuration Interaction Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9181-9188. | 1.1 | 21 |
| 6191 | Effects of Excitation Energy on the Autodetachment Lifetimes of Small Iodide-Doped ROH Clusters (R ₃ CH ⁺ , CH ₃ ⁺ , CH ₃ CH ₂ ⁺). <i>Journal of Physical Chemistry A</i> , 2012, 116, 2750-2757. | 1.1 | 9 |
| 6192 | Stereochemistry and Mechanism of the Ring-Opening Reaction of Cyclopropylenones with LiCu(Me) ₂ . <i>Organometallics</i> , 2012, 31, 7849-7854. | 1.1 | 7 |
| 6193 | Nonexponential Solid State ¹ H and ¹⁹ F Spin-Lattice Relaxation, Single-crystal X-ray Diffraction, and Isolated-Molecule and Cluster Electronic Structure Calculations in an Organic Solid: Coupled Methyl Group Rotation and Methoxy Group Libration in 4,4'-Dimethoxyoctafluorobiphenyl. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11946-11956. | 1.1 | 9 |
| 6194 | Mechanistic Studies of the CuH-Catalyzed Synthesis of $\hat{\pm}$ -Hydroxyallenes. <i>Organometallics</i> , 2012, 31, 8024-8030. | 1.1 | 11 |
| 6195 | Observation of the Inverse Trans Influence (ITI) in a Uranium(V) Imide Coordination Complex: An Experimental Study and Theoretical Evaluation. <i>Inorganic Chemistry</i> , 2012, 51, 6190-6199. | 1.9 | 67 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6196 | Anharmonic Vibrational Frequency Shifts upon Interaction of Phenol(+) with the Open Shell Ligand O_2 . The Performance of DFT Methods versus MP2. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1939-1949. | 1.1 | 5 |
| 6197 | Large Tunneling Effect on the Hydrogen Transfer in Bis(μ -oxo)dicopper Enzyme: A Theoretical Study. <i>Journal of the American Chemical Society</i> , 2012, 134, 3524-3531. | 6.6 | 18 |
| 6198 | Toward Rational Design of Metal-Organic Frameworks for Sensing Applications: Efficient Calculation of Adsorption Characteristics in Zero Loading Regime. <i>Journal of Physical Chemistry C</i> , 2012, 116, 3025-3033. | 1.5 | 48 |
| 6199 | Accuracy of Calculations of Heats of Reduction/Hydrogenation: Application to Some Small Ring Systems. <i>Journal of Organic Chemistry</i> , 2012, 77, 10393-10398. | 1.7 | 14 |
| 6200 | Calculating Off-Site Excitations in Symmetric Donor-Acceptor Systems via Time-Dependent Density Functional Theory with Range-Separated Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2661-2668. | 2.3 | 34 |
| 6201 | Theoretical Investigation of the Reaction of Mn^+ with Ethylene Oxide. <i>Journal of Physical Chemistry A</i> , 2012, 116, 512-519. | 1.1 | 2 |
| 6202 | Efficient Calculations of Dispersion Energies for Nanoscale Systems from Coupled Density Response Functions. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1963-1969. | 2.3 | 46 |
| 6203 | Fascinating effect of dehydrogenation on the transport properties of N-heteropentacenes: transformation from p- to n-type semiconductor. <i>Journal of Materials Chemistry</i> , 2012, 22, 18181. | 6.7 | 44 |
| 6204 | Influence of Sequential Thiolate Oxidation on a Nitrile Hydratase Mimic Probed by Multiedge X-ray Absorption Spectroscopy. <i>Inorganic Chemistry</i> , 2012, 51, 6032-6045. | 1.9 | 24 |
| 6205 | Osmium-Germanium and Osmium-Germanium-Gold Carbonyl Cluster Complexes: Syntheses, Structures, Bonding, and Reactivity. <i>Organometallics</i> , 2012, 31, 8639-8646. | 1.1 | 18 |
| 6206 | Benchmark Database for Ylidic Bond Dissociation Energies and Its Use for Assessments of Electronic Structure Methods. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2824-2834. | 2.3 | 62 |
| 6207 | Dual-Copper Catalytic Site Formed in CuMFI Zeolite Makes Effective Activation of Ethane Possible Even at Room Temperature. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10680-10691. | 1.5 | 14 |
| 6208 | DFT Studies on Gold-Catalyzed Cycloisomerization of 1,5-Enynes. <i>Organometallics</i> , 2012, 31, 4221-4227. | 1.1 | 29 |
| 6209 | C-H Bond Activation by Cationic Iridium(III) NHC Complexes: A Combined Experimental and Computational Study. <i>Organometallics</i> , 2012, 31, 1879-1887. | 1.1 | 29 |
| 6210 | Synthesis, characterization and quantum chemical ab initio calculations of new dimeric aminocyclodiphosph(V)azane and its Co(II), Ni(II) and Cu(II) complexes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 95, 414-422. | 2.0 | 18 |
| 6211 | Spectroscopic analysis of the interaction between thiazolo[2,3-b]pyrimidine analogues and bovine serum albumin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 690-697. | 2.0 | 7 |
| 6212 | Molecular structure investigation and spectroscopic studies on 2,3-difluorophenylboronic acid: A combined experimental and theoretical analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 97, 892-908. | 2.0 | 48 |
| 6213 | A dinuclear manganese(II) complex $\{[Na_2(H_2O)_4Mn_2(\mu_4-pmtz)_4(NCS)_2] \cdot xH_2O\}_n$ with 5-(pyrimidyl)tetrazolato bridges involved in 1D ladder-like chains: Synthesis, X-ray structure, magnetic properties and DFT calculations. <i>Polyhedron</i> , 2012, 42, 50-56. | 1.0 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6214 | Redox coupled-spin crossover in cobalt \hat{I}^2 -diketonate complexes: Structural, electrochemical and computational studies. <i>Polyhedron</i> , 2012, 42, 291-301. | 1.0 | 4 |
| 6215 | Photophysical properties of a fluorene- \hat{b} ipyridine copolymer and its complexes with europium. <i>Synthetic Metals</i> , 2012, 162, 35-43. | 2.1 | 23 |
| 6216 | Time-dependent density functional theory investigate the effect of arylacetylide chain length of cyclometalated Pt(II) complexes. <i>Synthetic Metals</i> , 2012, 162, 670-676. | 2.1 | 12 |
| 6217 | Thermal behavior of 1,7-diamino-1,7-dinitrimino-2,4,6-trinitro-2,4,6-triazaheptane. <i>Thermochimica Acta</i> , 2012, 541, 25-30. | 1.2 | 10 |
| 6218 | DFT studies of unique stereoelectronic effects of substituents on divergent reaction pathways of methylenecyclobutanone radical cations. <i>Tetrahedron</i> , 2012, 68, 5564-5571. | 1.0 | 3 |
| 6219 | Scandium-Decorated MOF-5 as Potential Candidates for Room-Temperature Hydrogen Storage: A Solution for the Clustering Problem in MOFs. <i>Journal of Physical Chemistry C</i> , 2012, 116, 17336-17342. | 1.5 | 50 |
| 6220 | Direct dynamics simulation of dioxetane formation and decomposition via the singlet \hat{A} - \hat{O} - \hat{O} - $\hat{C}H_2$ - $\hat{C}H_2$ -biradical: Non-RRKM dynamics. <i>Journal of Chemical Physics</i> , 2012, 137, 044305. | 1.2 | 22 |
| 6221 | Basis Set Recommendations for DFT Calculations of Gas-Phase Optical Rotation at Different Wavelengths. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4425-4433. | 2.3 | 26 |
| 6222 | Mechanism of the $MeReO_3$ -Catalyzed Deoxygenation of Epoxides. <i>Organometallics</i> , 2012, 31, 6139-6147. | 1.1 | 39 |
| 6223 | BDE261: A Comprehensive Set of High-Level Theoretical Bond Dissociation Enthalpies. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4975-4986. | 1.1 | 62 |
| 6224 | Theoretical Study of the Electronic Spectra of Small Molecules That Incorporate Analogues of the Copper-Cysteine Bond. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8507-8514. | 1.1 | 7 |
| 6225 | Gas-Phase Retinal Spectroscopy: Temperature Effects Are But a Mirage. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 908-912. | 2.1 | 19 |
| 6226 | Effects of Dispersion in Density Functional Based Quantum Mechanical/Molecular Mechanical Calculations on Cytochrome P450 Catalyzed Reactions. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4637-4645. | 2.3 | 85 |
| 6227 | State-of-the-art and challenges in theoretical simulations of heterogeneous catalysis at the microscopic level. <i>Catalysis Science and Technology</i> , 2012, 2, 2405. | 2.1 | 38 |
| 6228 | Influence of the Anchoring Modes on the Electronic and Photovoltaic Properties of \hat{D} - \hat{A} Dyes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 16876-16884. | 1.5 | 53 |
| 6229 | An Extension and Further Validation of an All-Atomistic Force Field for Biological Membranes. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2938-2948. | 2.3 | 408 |
| 6230 | Biphasic water splitting by osmocene. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 11558-11563. | 3.3 | 41 |
| 6231 | Comparative Study of Single and Double Hybrid Density Functionals for the Prediction of 3d Transition Metal Thermochemistry. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4102-4111. | 2.3 | 69 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6232 | Electronic Structure and Optical Properties of an Alternated Fluorene-Benzo-thiadiazole Copolymer: Interplay between Experimental and Theoretical Data. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3681-3690. | 1.1 | 26 |
| 6233 | How Evenly Can Approximate Density Functionals Treat the Different Multiplicities and Ionization States of 4d Transition Metal Atoms?. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4112-4126. | 2.3 | 37 |
| 6234 | Unraveling the Mechanisms of Carboxyl Ester Bond Hydrolysis Catalyzed by a Vanadate Anion. <i>Inorganic Chemistry</i> , 2012, 51, 9619-9628. | 1.9 | 7 |
| 6235 | Connecting [NiFe]- and [FeFe]-Hydrogenases: Mixed-Valence Nickel-Iron Dithiolates with Rotated Structures. <i>Inorganic Chemistry</i> , 2012, 51, 8931-8941. | 1.9 | 41 |
| 6236 | Evidence for the Formation of a Mo-H Intermediate in the Catalytic Cycle of Formate Dehydrogenase. <i>Inorganic Chemistry</i> , 2012, 51, 8331-8339. | 1.9 | 37 |
| 6237 | Modeling Surface Passivation of ZnS Quantum Dots. <i>Journal of Physical Chemistry C</i> , 2012, 116, 2740-2750. | 1.5 | 27 |
| 6238 | Study of Prepolymerization Complex Formation in the Synthesis of Steroid-Based Molecularly Imprinted Polymers. <i>Analytical Chemistry</i> , 2012, 84, 4481-4488. | 3.2 | 18 |
| 6239 | Improved Electronic Excitation Energies from Shape-Corrected Semilocal Kohn-Sham Potentials. <i>Physical Review Letters</i> , 2012, 108, 253005. | 2.9 | 35 |
| 6240 | Molecular Dynamics and Umbrella Sampling Study of Stabilizing Factors in Cyclic Peptide-Based Nanotubes. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9922-9933. | 1.2 | 35 |
| 6241 | Vibrational Circular Dichroism versus Optical Rotation Dispersion and Electronic Circular Dichroism for diastereomers: the stereochemistry of 3-(1-hydroxyethyl)-1-(3-phenylpropanoyl)-azetidin-2-one. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8562. | 1.3 | 30 |
| 6242 | Overcoming Low Orbital Overlap and Triplet Instability Problems in TDDFT. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9783-9789. | 1.1 | 190 |
| 6243 | Vibrationally assisted electron transfer mechanism of olfaction: myth or reality?. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 13861. | 1.3 | 53 |
| 6244 | Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. <i>Journal of Chemical Physics</i> , 2012, 136, 174103. | 1.2 | 99 |
| 6245 | Thermodynamic and Kinetic Hydricity of Ruthenium(II) Hydride Complexes. <i>Journal of the American Chemical Society</i> , 2012, 134, 15743-15757. | 6.6 | 117 |
| 6246 | Atomic $\langle i \rangle C \langle /i \rangle \langle sub \rangle 6 \langle /sub \rangle$ dispersion coefficients: a four-component relativistic Kohn-Sham study. <i>Molecular Physics</i> , 2012, 110, 2535-2541. | 0.8 | 13 |
| 6247 | Solvated First-Principles Excited-State Charge-Transfer Dynamics with Time-Dependent Polarizable Continuum Model and Solvent Dielectric Relaxation. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2898-2904. | 2.1 | 40 |
| 6248 | Specific His ₆ -tag Attachment to Metal-Functionalized Polymersomes Relies on Molecular Recognition. <i>Journal of Physical Chemistry B</i> , 2012, 116, 10113-10124. | 1.2 | 19 |
| 6249 | Inorganic photoisomerization: the case study of rhenium(i) complexes. <i>Dalton Transactions</i> , 2012, 41, 13191. | 1.6 | 28 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6250 | A Density Functional with Spherical Atom Dispersion Terms. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4989-5007. | 2.3 | 463 |
| 6251 | Reductive Eliminations from λ^3 -Iodanes: Understanding Selectivity and the Crucial Role of the Hypervalent Bond. <i>Organic Letters</i> , 2012, 14, 3830-3833. | 2.4 | 50 |
| 6252 | Empirical Correction of Nondynamical Correlation Energy for Density Functionals. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9969-9978. | 1.1 | 16 |
| 6253 | Thermal Decomposition Mechanism of 1-Ethyl-3-methylimidazolium Bromide Ionic Liquid. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5867-5876. | 1.1 | 57 |
| 6254 | Sorbitol Hydrogenolysis Over Ni, Pt and Ru Supported on NaY. <i>Topics in Catalysis</i> , 2012, 55, 897-907. | 1.3 | 42 |
| 6255 | Exploring the Limits of Density Functional Approximations for Interaction Energies of Molecular Precursors to Organic Electronics. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4305-4316. | 2.3 | 38 |
| 6256 | Imidazole Based Ruthenium(IV) Complexes as Highly Efficient Bifunctional Catalysts for the Redox Isomerization of Allylic Alcohols in Aqueous Medium: Water as Cooperating Ligand. <i>ACS Catalysis</i> , 2012, 2, 2087-2099. | 5.5 | 55 |
| 6257 | Mechanistic Study of the Synthesis of CdSe Nanocrystals: Release of Selenium. <i>Journal of the American Chemical Society</i> , 2012, 134, 1400-1403. | 6.6 | 53 |
| 6258 | Experimental and theoretical investigation of the oxidative carbonylation of toluene to toluic acid catalyzed by palladium(II) in the presence of vanadium and molecular oxygen. <i>Journal of Molecular Catalysis A</i> , 2012, 361-362, 91-97. | 4.8 | 5 |
| 6259 | Density functional theory and vibrational studies of mianserin and its hydrochloride and hydrobromide salts. <i>Journal of Molecular Structure</i> , 2012, 1021, 53-62. | 1.8 | 8 |
| 6260 | The structures of pentanoyl chloride, $\text{CH}_3(\text{CH}_2)_3\text{COCl}$, contained in supersonic expansions of argon gas. <i>Journal of Molecular Structure</i> , 2012, 1021, 29-33. | 1.8 | 1 |
| 6261 | Synthesis, crystal structure and redox properties of dihydropyrazole-bridged ferrocene-based derivatives. <i>Journal of Molecular Structure</i> , 2012, 1024, 40-46. | 1.8 | 13 |
| 6262 | Unusual hydrogen-bonding aggregation in 4-amino-1-(2-carboxyethyl)pyridinium bromide hemihydrate. <i>Journal of Molecular Structure</i> , 2012, 1026, 150-158. | 1.8 | 5 |
| 6263 | Conformational preferences for some 3-(4- ϵ^2 -substituted phenylsulfonyl)-1-methyl-2-piperidones through spectroscopic and theoretical studies. <i>Journal of Molecular Structure</i> , 2012, 1028, 97-106. | 1.8 | 5 |
| 6264 | Diastereomerism in tetranuclear copper(II) complexes of a phenol based C_2O_2 -compartmental ligand. <i>Inorganic Chemistry Communication</i> , 2012, 23, 113-116. | 1.8 | 12 |
| 6265 | Synthesis and studies of covalently linked meso-furyl boron-dipyrrromethene-ferrocene conjugates. <i>Journal of Organometallic Chemistry</i> , 2012, 697, 65-73. | 0.8 | 35 |
| 6266 | Transition metal compounds containing alkynylsilyl groups M^{II} complexes with a metal-silicon bond. <i>Journal of Organometallic Chemistry</i> , 2012, 705, 59-69. | 0.8 | 11 |
| 6267 | DFT studies on the mechanism of the conversion of thiols into disulfides and dihydrogen catalyzed by $\text{CpMn}(\text{CO})_3$ complex. <i>Journal of Organometallic Chemistry</i> , 2012, 706-707, 89-98. | 0.8 | 15 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6268 | Structural motifs, thermodynamic properties, bonding and aromaticity of sandwich complexes formed by alkaline earth metals with pentafulvene. A theoretical approach. <i>Journal of Organometallic Chemistry</i> , 2012, 708-709, 10-17. | 0.8 | 8 |
| 6269 | The solid-state, solution and gas-phase interactions of diphosphane monooxide spacers with heavier group 8,9 transition metals and gallium in novel organometallic assemblies: An experimental and computational study. <i>Journal of Organometallic Chemistry</i> , 2012, 714, 22-31. | 0.8 | 2 |
| 6270 | Synthesis and optical properties of spirobi(dithienometalole)s and spirobi(dithienothiametalline)s. <i>Journal of Organometallic Chemistry</i> , 2012, 710, 53-58. | 0.8 | 26 |
| 6271 | 1,1'-Bis(diphenylphosphino)ferrocene bridging two mono(cyclopentadienyl) cobalt moieties: Synthesis, structure, electrochemistry and DFT studies. <i>Journal of Organometallic Chemistry</i> , 2012, 712, 52-56. | 0.8 | 4 |
| 6272 | Turn-on colorimetric sensing of fluoride ions by a cationic triarylborane bearing benzothiazolium. <i>Journal of Organometallic Chemistry</i> , 2012, 713, 89-95. | 0.8 | 26 |
| 6273 | Ru(II)-halide-carbonyl complexes of naphthylazoimidazoles: Synthesis, spectra, electrochemistry, catalytic activity and electronic structure. <i>Journal of Organometallic Chemistry</i> , 2012, 716, 129-137. | 0.8 | 22 |
| 6274 | Quantum chemical study on first hyperpolarizabilities of mono- and bimetal Pt(II) diimine complexes. <i>Journal of Organometallic Chemistry</i> , 2012, 718, 1-7. | 0.8 | 9 |
| 6275 | Quantum chemical study of PtF and PtCl ($n=1-6$) complexes: An investigation of superhalogen properties. <i>Computational and Theoretical Chemistry</i> , 2012, 979, 119-127. | 1.1 | 11 |
| 6276 | The effect of ionization and deprotonation of guanine on the formation of base pairs. <i>Computational and Theoretical Chemistry</i> , 2012, 980, 23-31. | 1.1 | 3 |
| 6277 | Theoretical investigation of the conducting properties of substituted phosphole oligomers. <i>Computational and Theoretical Chemistry</i> , 2012, 980, 68-72. | 1.1 | 7 |
| 6278 | Interaction of gold nanoclusters of different size with adenine: A density functional theory study of neutral, anionic and cationic forms of [adenine+(Au) $_n$] $_n=3,6,9,12$ complexes. <i>Computational and Theoretical Chemistry</i> , 2012, 984, 93-101. | 1.1 | 14 |
| 6279 | Validating empirical force fields for molecular-level simulation of cellulose dissolution. <i>Computational and Theoretical Chemistry</i> , 2012, 984, 119-127. | 1.1 | 24 |
| 6280 | Theoretical investigation of the static (dynamic) polarizability and second hyperpolarizability of DAAD quadrupolar push-pull molecules. A comparison among HF (TD-HF), DFT (TD-B3LYP), and MP2 (TD-MP2) methods. <i>Computational and Theoretical Chemistry</i> , 2012, 985, 72-79. | 1.1 | 24 |
| 6281 | Exploring the unexpected pyridine- and 4,4'-bipyridine-catalyzed isomerization of maleic acid: A DFT approach. <i>Computational and Theoretical Chemistry</i> , 2012, 988, 63-74. | 1.1 | 5 |
| 6282 | Metal salts reduction during parylenes polymerization. <i>Computational and Theoretical Chemistry</i> , 2012, 991, 56-65. | 1.1 | 2 |
| 6283 | Theoretical investigation on the Pt($\delta^+\delta^+$)-catalyzed [3+2] cycloaddition reactions of propargyl ether derivatives with <i>n</i> -butyl vinyl ether. <i>Computational and Theoretical Chemistry</i> , 2012, 992, 97-102. | 1.1 | 9 |
| 6284 | A DFT study on the structures and stabilities of As-doped Si_n^{-1} ($n=2-15$) clusters. <i>Computational and Theoretical Chemistry</i> , 2012, 992, 134-141. | 1.1 | 3 |
| 6285 | DFT study on Pt(II)-catalyzed tandem reaction of propargylic ester. <i>Computational and Theoretical Chemistry</i> , 2012, 993, 125-130. | 1.1 | 1 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6286 | Inhibition effect of 4-amino-antipyrine on the corrosion of copper in 3 wt.% NaCl solution. <i>Corrosion Science</i> , 2012, 57, 270-278. | 3.0 | 108 |
| 6287 | Libxc: A library of exchange and correlation functionals for density functional theory. <i>Computer Physics Communications</i> , 2012, 183, 2272-2281. | 3.0 | 419 |
| 6288 | A new meta-GGA exchange functional based on an improved constraint-based GGA. <i>Chemical Physics Letters</i> , 2012, 543, 179-183. | 1.2 | 44 |
| 6289 | Theoretical study of the four isomers of [Siw11o39]8 ⁺ : Structure, stability and physical properties. <i>Comptes Rendus Chimie</i> , 2012, 15, 143-151. | 0.2 | 11 |
| 6290 | First principles investigation of the atomic structure and magnetic properties of copper hydroxide acetate. <i>Comptes Rendus Chimie</i> , 2012, 15, 202-208. | 0.2 | 5 |
| 6291 | Electronic fine structure calculation of [Gd(DOTA)(H ₂ O)] ³⁺ using LF-DFT: The zero field splitting. <i>Comptes Rendus Chimie</i> , 2012, 15, 250-254. | 0.2 | 13 |
| 6292 | Structures and spectral properties of heteroleptic copper (I) complexes: A theoretical study based on density functional theory. <i>Comptes Rendus Chimie</i> , 2012, 15, 255-266. | 0.2 | 9 |
| 6293 | Spin-orbit and modified Becke-Johnson potential effects on the electronic properties of bulk Ge: A density functional theory study. <i>Computational Materials Science</i> , 2012, 54, 37-42. | 1.4 | 17 |
| 6294 | First-principles study of Fe-based superconductors: A comparison of screened hybrid functional with gradient corrected functional. <i>Computational Materials Science</i> , 2012, 55, 284-294. | 1.4 | 4 |
| 6295 | Protonated o-semiquinone radical as a mimetic of the humic acids native radicals: A DFT approach to the molecular structure and EPR properties. <i>Geochimica Et Cosmochimica Acta</i> , 2012, 86, 384-391. | 1.6 | 13 |
| 6296 | Theoretical study of nitrogen-rich CN ₃ ⁻ anion and related salts M+[CN ₃] ⁻ (M = Li, Na, K). <i>RSC Advances</i> , 2012, 2, 11764. | 1.7 | 17 |
| 6297 | Structure of AgI-doped Ge ¹¹ In ¹¹ S glasses: Experiment, reverse Monte Carlo modelling, and density functional calculations. <i>Journal of Solid State Chemistry</i> , 2012, 192, 7-15. | 1.4 | 18 |
| 6298 | Electronic structures and second-order nonlinear optical properties of a series of functionalized Sc ₃ N@C ₈₀ derivatives. <i>Computational and Theoretical Chemistry</i> , 2012, 996, 51-56. | 1.1 | 1 |
| 6300 | Organocatalytic Activation of Polycyclic Aromatic Compounds for Asymmetric Diels-Alder Reactions. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 10271-10274. | 7.2 | 79 |
| 6301 | Use of Melem as a Nucleophilic Reagent to Form the Triphthalimide C ₆ N ₇ (phthal) ₃ New Targets and Prospects. <i>Chemistry - A European Journal</i> , 2012, 18, 12052-12058. | 1.7 | 28 |
| 6302 | Direct Detection of Key Intermediates in Rhodium(I)-Catalyzed [2+2+2] Cycloadditions of Alkynes by ESI-MS. <i>Chemistry - A European Journal</i> , 2012, 18, 13097-13107. | 1.7 | 37 |
| 6303 | Disclosing the Structure/Activity Correlation in Trivalent Boron-Containing Compounds: A Tendency Map. <i>Chemistry - A European Journal</i> , 2012, 18, 12794-12802. | 1.7 | 69 |
| 6304 | Predicting the Enantioselectivity of the Copper-Catalysed Cyclopropanation of Alkenes by Using Quantitative Quadrant Diagram Representations of the Catalysts. <i>Chemistry - A European Journal</i> , 2012, 18, 14026-14036. | 1.7 | 39 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6305 | Radical Localization in a Series of Symmetric Ni ^{II} Complexes with Oxidized Salen Ligands. Chemistry - A European Journal, 2012, 18, 14117-14127. | 1.7 | 76 |
| 6306 | A Spectroscopic and Computational Study of a Photoinduced Cross-Dehydrogenative Coupling Reaction of a Stable Semiquinone Radical. Chemistry - A European Journal, 2012, 18, 13605-13608. | 1.7 | 3 |
| 6307 | Supramolecular Assembly of Diplatinum Species through Weak Pt ^{II} ...Pt ^{II} Intermolecular Interactions: A Combined Experimental and Computational Study. Chemistry - A European Journal, 2012, 18, 13787-13799. | 1.7 | 15 |
| 6308 | Synthesis and Characterization of Rhenabenzyne Complexes. Chemistry - A European Journal, 2012, 18, 14128-14139. | 1.7 | 36 |
| 6309 | Molecular Description of the Propagation of Chirality from Molecules to Complex Systems: Different Mechanisms Controlled by Hydrophobic Interactions. Chemistry - A European Journal, 2012, 18, 14680-14688. | 1.7 | 18 |
| 6310 | Analysis of the Electronic Circular Dichroism Spectrum of (Λ)-[9](2,5)Pyridinophane. Chirality, 2012, 24, 994-1004. | 1.3 | 6 |
| 6311 | Redox-Active Guanidine Ligands with Pyridine and <i>p</i> -Benzoquinone Backbones. European Journal of Inorganic Chemistry, 2012, 2012, 4833-4845. | 1.0 | 36 |
| 6312 | [2.2]Paracyclophanediyl diphosphane Complexes of Gold. European Journal of Inorganic Chemistry, 2012, 2012, 5033-5042. | 1.0 | 32 |
| 6313 | Proton shuffling in acid/base-catalyzed enolizations: a computational study. Journal of Physical Organic Chemistry, 2012, 25, 1336-1342. | 0.9 | 3 |
| 6314 | Molecular and crystal structure of (pyrazin-1-ium-1-yl)(perfluoropyridin-4-yl) and (4,4'-bipyridin-1-ium-1-yl)(perfluoropyridin-4-yl)amides. Journal of Structural Chemistry, 2012, 53, 948-953. | 0.3 | 0 |
| 6315 | Theoretical study of the reductive decomposition of 1,3-propane sultone: SEI forming additive in lithium-ion batteries. RSC Advances, 2012, 2, 5439. | 1.7 | 48 |
| 6316 | Accurate Hydrogen Positions in Organic Crystals: Assessing a Quantum-Chemical Aide. Crystal Growth and Design, 2012, 12, 1014-1021. | 1.4 | 68 |
| 6317 | A computational study of the enantioselective addition of <i>n</i> -BuLi to benzaldehyde in the presence of a chiral lithium N,P amide. Organic and Biomolecular Chemistry, 2012, 10, 2807. | 1.5 | 12 |
| 6318 | On the intrinsic photophysics of indigo: a time-resolved photoelectron spectroscopy study of the indigo carmine dianion. Physical Chemistry Chemical Physics, 2012, 14, 16155. | 1.3 | 25 |
| 6319 | Titanium(IV) Trifluoromethyl Complexes: New Perspectives on Bonding from Organometallic Fluorocarbon Chemistry. Organometallics, 2012, 31, 1484-1499. | 1.1 | 37 |
| 6320 | Theoretical infrared and electronic absorption spectra of C ₁₆ H ₁₀ isomers, their ions and doubly ions. Monthly Notices of the Royal Astronomical Society, 2012, 425, 490-505. | 1.6 | 5 |
| 6321 | Structurally modified 1,10-phenanthroline based fluorophores for specific sensing of Ni ²⁺ and Cu ²⁺ ions. Dalton Transactions, 2012, 41, 5769. | 1.6 | 25 |
| 6322 | Accurate evaluation of the resonance energies of benzene and pyridine via cyclic reference state. Physical Chemistry Chemical Physics, 2012, 14, 15888. | 1.3 | 8 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6323 | Platinum Clusters on Vacancy-Type Defects of Nanometer-Sized Graphene Patches. <i>Molecules</i> , 2012, 17, 7941-7960. | 1.7 | 15 |
| 6324 | Resolution of a Challenge for Solvation Modeling: Calculation of Dicarboxylic Acid Dissociation Constants Using Mixed Discrete-Continuum Solvation Models. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1437-1442. | 2.1 | 76 |
| 6325 | Dioxygen Activation by a Non-Heme Iron(II) Complex: Theoretical Study toward Understanding Ferric-Superoxo Complexes. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 915-926. | 2.3 | 65 |
| 6327 | Adsorption of Hydrocarbons in Metal-Organic Frameworks: A Force Field Benchmark on the Example of Benzene in Metal-Organic Framework 5. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15369-15377. | 1.5 | 14 |
| 6329 | Localized optimized orbitals, coupled cluster theory, and chiroptical response properties. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7830. | 1.3 | 26 |
| 6330 | Oxygen Activation on Nanometer-Size Gold Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15992-16000. | 1.5 | 39 |
| 6331 | Iron-catalysed transformation of molecular dinitrogen into silylamine under ambient conditions. <i>Nature Communications</i> , 2012, 3, 1254. | 5.8 | 118 |
| 6332 | DFT Studies on the Mechanisms of the Platinum-Catalyzed Diboration of Acyclic Unsaturated Carbonyl Compounds. <i>Organometallics</i> , 2012, 31, 3410-3425. | 1.1 | 72 |
| 6333 | Ruthenium(II) Arene Complexes with Asymmetrical Guanidinate Ligands: Synthesis, Characterization, and Application in the Base-Free Catalytic Isomerization of Allylic Alcohols. <i>Organometallics</i> , 2012, 31, 8301-8311. | 1.1 | 40 |
| 6334 | Computations of 36 Tautomer/Isomer Equilibria of Different Lactams. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6885-6893. | 1.1 | 11 |
| 6335 | Photoelectron Spectroscopy of Palladium(I) Dimers with Bridging Allyl Ligands. <i>Organometallics</i> , 2012, 31, 8571-8576. | 1.1 | 5 |
| 6336 | A qualitative failure of B3LYP for textbook organic reactions. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7170. | 1.3 | 62 |
| 6337 | Quantum Mechanical Continuum Solvation Models for Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9122-9129. | 1.2 | 225 |
| 6338 | An interpretation of the absorption and emission spectra of the gold dimer using modern theoretical tools. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8732. | 1.3 | 22 |
| 6339 | Theoretical and numerical assessments of spin-flip time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2012, 136, 024107. | 1.2 | 66 |
| 6340 | Iron-Centered Ten-Vertex Germanium Clusters: The Ubiquity of Low Energy Pentagonal Prismatic Structures with Various Skeletal Electron Counts. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9197-9204. | 1.1 | 17 |
| 6341 | XYG3 and XYGJ-OS performances for noncovalent binding energies relevant to biomolecular structures. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12554. | 1.3 | 32 |
| 6342 | Density functional theory study of CO ₂ capture with transition metal oxides and hydroxides. <i>Journal of Chemical Physics</i> , 2012, 136, 064516. | 1.2 | 26 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6343 | Studies of 1,2-Dihalo Shifts in Carbon \rightarrow Carbon, Carbon \rightarrow Silicon, and Silicon \rightarrow Silicon Systems: A Computational Study. <i>Organometallics</i> , 2012, 31, 8426-8436. | 1.1 | 5 |
| 6344 | The Nature of Transannular Interactions in E4N4 and E82+ (E = S, Se). <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4249-4258. | 2.3 | 13 |
| 6346 | Complete basis set, hybrid-density functional theory study, and natural bond orbital interpretations of the conformational behavior of halocarbonyl, thiocarbonyl, and selenocarbonyl isocyanates. <i>Canadian Journal of Chemistry</i> , 2012, 90, 333-343. | 0.6 | 1 |
| 6347 | Convergence of Electronic Structure with the Size of the QM Region: Example of QM/MM NMR Shieldings. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2260-2271. | 2.3 | 111 |
| 6348 | A new series of isorecticular copper-based metal \rightarrow organic frameworks containing non-linear linkers with different group 14 central atoms. <i>Journal of Materials Chemistry</i> , 2012, 22, 10294. | 6.7 | 9 |
| 6349 | Vapors from Ionic Liquids: Reconciling Simulations with Mass Spectrometric Data. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3435-3441. | 2.1 | 51 |
| 6350 | Spiroligozymes for Transesterifications: Design and Relationship of Structure to Activity. <i>Journal of the American Chemical Society</i> , 2012, 134, 18345-18353. | 6.6 | 41 |
| 6351 | Density functional theory with fractional orbital occupations. <i>Journal of Chemical Physics</i> , 2012, 136, 154104. | 1.2 | 127 |
| 6353 | Force Field Development for Actinyl Ions via Quantum Mechanical Calculations: An Approach to Account for Many Body Solvation Effects. <i>Journal of Physical Chemistry B</i> , 2012, 116, 10885-10897. | 1.2 | 38 |
| 6354 | Kinetics and mechanism of the reactions of Au(III) complexes with some biologically relevant molecules. <i>Dalton Transactions</i> , 2012, 41, 3633. | 1.6 | 35 |
| 6355 | The high yield synthesis and characterization of gold nanoparticles with superior stability and their catalytic activity. <i>CrystEngComm</i> , 2012, 14, 7600. | 1.3 | 43 |
| 6356 | Cyclopentadienyl chromium diimine and pyridine-imine complexes: ligand-based radicals and metal-based redox chemistry. <i>Dalton Transactions</i> , 2012, 41, 7920. | 1.6 | 13 |
| 6357 | Experimental and Theoretical Approach to Aggregation Behavior of New Di-N-Oxide Surfactants in an Aquatic Environment. <i>Journal of Physical Chemistry B</i> , 2012, 116, 14324-14332. | 1.2 | 14 |
| 6358 | Cu(I)/TF-Biphos Catalyzed Reactions of Alkylidene Bisphosphates and Alkylidene Malonates with Azomethine Ylides: Michael Addition versus 1,3-Dipolar Cycloaddition. <i>Organometallics</i> , 2012, 31, 7870-7876. | 1.1 | 44 |
| 6360 | Selective TDDFT with automatic removal of ghost transitions: application to a perylene-dye-sensitized solar cell model. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8608. | 1.3 | 13 |
| 6361 | Can Aromatic π -Clouds Complex Divalent Germanium and Tin Compounds? A DFT Study. <i>Organometallics</i> , 2012, 31, 1605-1617. | 1.1 | 26 |
| 6362 | Linear-Response and Real-Time Time-Dependent Density Functional Theory Studies of Core-Level Near-Edge X-Ray Absorption. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3284-3292. | 2.3 | 192 |
| 6363 | Catalyst Chelation Effects in Organocatalyzed Ring-Opening Polymerization of Lactide. <i>ACS Macro Letters</i> , 2012, 1, 19-22. | 2.3 | 64 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6364 | Chirality in Copper Nanoalloy Clusters. <i>Journal of Physical Chemistry C</i> , 2012, 116, 330-335. | 1.5 | 23 |
| 6366 | Conformational behavior of peracetylated β -D-mannopyranosyl methanesulfonamide: implications for the mechanism of sulfonamidoglycosylation of carbohydrate derivatives. <i>Carbohydrate Research</i> , 2012, 361, 182-188. | 1.1 | 6 |
| 6367 | Aromaticity of heptafulvene charge transfer complexes with lithium and caesium atoms: A computational approach. <i>Computational and Theoretical Chemistry</i> , 2012, 998, 46-50. | 1.1 | 5 |
| 6368 | Hydrogen-deuterium exchange in hydride chemistry: Dihydrogen bonded complexes as key intermediates. <i>Computational and Theoretical Chemistry</i> , 2012, 998, 129-140. | 1.1 | 18 |
| 6369 | Possible dimers of hypochlorous acid (HOCl) arising from hydrogen- and halogen-bond interactions. <i>Computational and Theoretical Chemistry</i> , 2012, 999, 48-54. | 1.1 | 10 |
| 6370 | Theoretical studies on the spectroscopic properties of a series of halide Zinc (II) complexes with pyridinylimine and pyridinylmethylamine derivatives. <i>Synthetic Metals</i> , 2012, 162, 2138-2148. | 2.1 | 7 |
| 6371 | Reaction products and mechanism of the regioselective oxidation of N-phenylmorpholine by ozone. <i>Tetrahedron</i> , 2012, 68, 8267-8275. | 1.0 | 16 |
| 6372 | Synthesis and reactivity of enediyne-nucleobase hybrids: effect of intramolecular π -stacking. <i>Tetrahedron</i> , 2012, 68, 8600-8611. | 1.0 | 9 |
| 6373 | Substituent effect of fluorine ligand on spectroscopic properties of Pt(N ^C N)Cl complexes, a theoretical study. <i>Organic Electronics</i> , 2012, 13, 2568-2574. | 1.4 | 18 |
| 6374 | Experimental (FT-IR and FT-RS) and theoretical (QC-DFT) studies of vibrational modes and molecular structure of new low-temperature phases of [Ru(NH ₃) ₆](BF ₄) ₃ and [Ru(NH ₃) ₆](ClO ₄) ₃ . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 98, 132-141. | 2.0 | 4 |
| 6375 | Molecular structure, vibrational, UV, NMR, hyperpolarizability, NBO and HOMO-LUMO analysis of Pteridine-2,4-dione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 99, 292-302. | 2.0 | 11 |
| 6376 | Interaction of alkali, alkaline earth and transition metal ions with a ketocyanine dye: A comparative electronic spectroscopic study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 99, 37-45. | 2.0 | 8 |
| 6377 | Chelation of a proton by oxidized diphosphines. <i>Journal of Organometallic Chemistry</i> , 2012, 721-722, 124-129. | 0.8 | 4 |
| 6378 | Theoretical characterization of a class of orange dopants for white-light-emitting single polymers. <i>Materials Chemistry and Physics</i> , 2012, 135, 965-972. | 2.0 | 0 |
| 6379 | Theoretical studies on the mechanism of oxazole with CO ₂ catalyzed by gold(I) complexes. <i>Journal of Molecular Catalysis A</i> , 2012, 363-364, 31-40. | 4.8 | 14 |
| 6380 | Computational Study on a HS ⁻ Sensing Reaction Utilizing a Pyrylium Derivative. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5420-5427. | 1.1 | 8 |
| 6381 | Theoretical prediction on the structures and stability of the noble-gas containing anions FN _g CC ⁻ (N _g =He, Ar, Kr, and Xe). <i>Journal of Chemical Physics</i> , 2012, 137, 194303. | 1.2 | 15 |
| 6382 | Modular electron donor group tuning of frontier energy levels in diarylamino-fluorenone push-pull molecules. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11961. | 1.3 | 26 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6383 | Superatomic orbitals in sixteen-coordinate M@Li ₁₆ bonded by metallic bonds. <i>Nanoscale</i> , 2012, 4, 2567. | 2.8 | 12 |
| 6384 | Optimized Structure and Vibrational Properties by Error Affected Potential Energy Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4204-4215. | 2.3 | 22 |
| 6385 | The prevalence of isocloso deltahedra in low-energy hypoelectronic metalladecaboranes with a single metal vertex: manganese and rhenium derivatives. <i>Dalton Transactions</i> , 2012, 41, 7073. | 1.6 | 13 |
| 6386 | Mechanisms of Organocatalytic Amidation and Trans-Esterification of Aromatic Esters As a Model for the Depolymerization of Poly(ethylene) Terephthalate. <i>Journal of Physical Chemistry A</i> , 2012, 116, 12389-12398. | 1.1 | 73 |
| 6387 | A "hidden" role of amino and imino groups is unveiled during the micro-solvation study of three biomolecule groups in water. <i>New Journal of Chemistry</i> , 2012, 36, 1866. | 1.4 | 6 |
| 6388 | Transition levels of defects in ZnO: Total energy and Janak's theorem methods. <i>Journal of Chemical Physics</i> , 2012, 137, 054709. | 1.2 | 22 |
| 6389 | Correlated Ab Initio Quantum Chemical Study of the Interaction of the Na ⁺ , Mg ²⁺ , Ca ²⁺ , and Zn ²⁺ Ions with the Tautomers of Cytosine. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4987-4994. | 1.1 | 7 |
| 6390 | Symmetric Halogen Bonding Is Preferred in Solution. <i>Journal of the American Chemical Society</i> , 2012, 134, 5706-5715. | 6.6 | 159 |
| 6391 | Hypoelectronic Dirhenaboranes Having Eight to Twelve Vertices: Internal Versus Surface Rhenium-Rhenium Bonding. <i>Inorganic Chemistry</i> , 2012, 51, 7609-7616. | 1.9 | 27 |
| 6392 | Theoretical Determination of One-Electron Oxidation Potentials for Nucleic Acid Bases. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 5107-5123. | 2.3 | 72 |
| 6393 | Pyrolysis of 3-azidopropionitrile studied by UV photoelectron and matrix-isolation IR spectroscopies: Formation of ketenimine H ₂ C=C=NH. <i>Journal of Molecular Structure</i> , 2012, 1025, 151-159. | 1.8 | 5 |
| 6394 | Computational Studies of the Metal-Binding Site of the Wild-Type and the H46R Mutant of the Copper, Zinc Superoxide Dismutase. <i>Inorganic Chemistry</i> , 2012, 51, 5561-5568. | 1.9 | 12 |
| 6395 | Magnetostructural effects in ligand stabilized Pd ₁₃ clusters: a density functional theory study. <i>Nanoscale</i> , 2012, 4, 4138. | 2.8 | 17 |
| 6396 | Synthesis of Benzoindolines via a Copper-Catalyzed Reaction of 1-Bromoethynyl-(cyclopropylidene)methyl)arenes with N-Allylsulfonamide. <i>Advanced Synthesis and Catalysis</i> , 2012, 354, 3087-3094. | 2.1 | 22 |
| 6397 | The Effect of Side-Chain Length on the Solid-State Structure and Optoelectronic Properties of Fluorene-Benzothiadiazole Based Conjugated Polymers: A DFT Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10597-10606. | 1.1 | 20 |
| 6398 | Diruthenium(III,III) Ethynyl-phenyleneimine Molecular Wires: Preparation via On-Complex Schiff Base Condensation. <i>Inorganic Chemistry</i> , 2012, 51, 7561-7568. | 1.9 | 14 |
| 6399 | 1H-1,2,4-Triazole as solvent for imidazolium methanesulfonate. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11441. | 1.3 | 24 |
| 6400 | Synthesis and Characterization of 5-Nitro-2-nitratomethyl-1,2,3,4-tetrazole: A High Nitrogen Energetic Compound with Good Oxygen Balance. <i>Molecules</i> , 2012, 17, 5040-5049. | 1.7 | 27 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6401 | Exchangeâ€œCorrelation Functional with Good Accuracy for Both Structural and Energetic Properties while Depending Only on the Density and Its Gradient. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2310-2319. | 2.3 | 276 |
| 6402 | Outer-Sphere Contributions to the Electronic Structure of Type Zero Copper Proteins. <i>Journal of the American Chemical Society</i> , 2012, 134, 8241-8253. | 6.6 | 42 |
| 6403 | Metal binding selectivity of oxa-aza macrocyclic ligand: a DFT study of first- and second-row transition metal for four coordination systems. <i>Structural Chemistry</i> , 2012, 23, 1539-1545. | 1.0 | 7 |
| 6404 | Unexpected Disproportionation of Tetramethylethylenediamine-Supported Perchlorodisilane $\text{Cl}_3\text{SiSiCl}_3$. <i>Inorganic Chemistry</i> , 2012, 51, 8599-8606. | 1.9 | 47 |
| 6405 | Stereodynamics in Eight-Coordination; A 2D NMR Spectroscopic and Computational Study of the Exchange Process in $\text{ThCl}_4(\text{Me}_2\text{NCH}_2\text{CH}_2\text{NMe}_2)_2$. <i>Inorganic Chemistry</i> , 2012, 51, 10141-10147. | 1.9 | 3 |
| 6406 | A Multilevel Strategy for the Exploration of the Conformational Flexibility of Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1808-1819. | 2.3 | 35 |
| 6407 | Theoretical study of the bridging effect on the charge carrier transport properties of cyclooctatetrathiophene and its derivatives. <i>Journal of Materials Chemistry</i> , 2012, 22, 6907. | 6.7 | 50 |
| 6408 | Selectivity of bis-triazinyl bipyridine ligands for americium(III) in Am/Eu separation by solvent extraction. Part 1. Quantum mechanical study on the structures of BTBP complexes and on the energy of the separation. <i>Dalton Transactions</i> , 2012, 41, 14416. | 1.6 | 64 |
| 6409 | Range-Separated Exchange Functionals with Slater-Type Functions. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 901-907. | 2.3 | 107 |
| 6410 | Computational study on the decomposition of tetra-n-propyl zirconium for the chemical vapor deposition of zirconium carbide. <i>Korean Journal of Chemical Engineering</i> , 2012, 29, 1438-1443. | 1.2 | 4 |
| 6411 | General formulation of spin-flip time-dependent density functional theory using non-collinear kernels: Theory, implementation, and benchmarks. <i>Journal of Chemical Physics</i> , 2012, 136, 204103. | 1.2 | 188 |
| 6412 | Pressure induced insulator/half-metal/metal transition in a strongly correlated $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle$ -electron system. <i>Physical Review B</i> , 2012, 85, . | 1.1 | 10 |
| 6413 | Surface-enhanced Raman spectroscopy studies of organophosphorous model molecules and pesticides. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 15645. | 1.3 | 45 |
| 6414 | Complex Vibrational Analysis of an Antiferroelectric Liquid Crystal Based on Solid-State Oriented Quantum Chemical Calculations and Experimental Molecular Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7809-7821. | 1.1 | 10 |
| 6415 | Diruthenium(III,III) Bis(alkynyl) Compounds with Donor/Acceptor-Substituted geminal-Diethynylethene Ligands. <i>Inorganic Chemistry</i> , 2012, 51, 3261-3269. | 1.9 | 26 |
| 6416 | Assessment of density functional theory for iron(II) molecules across the spin-crossover transition. <i>Journal of Chemical Physics</i> , 2012, 137, 124303. | 1.2 | 94 |
| 6417 | Cation Coordination and Motion in a Poly(ethylene oxide)-Based Single Ion Conductor. <i>Macromolecules</i> , 2012, 45, 6230-6240. | 2.2 | 62 |
| 6418 | MOLECULAR BIOLOGY AT THE QUANTUM LEVEL: CAN MODERN DENSITY FUNCTIONAL THEORY FORGE THE PATH?. <i>Nano LIFE</i> , 2012, 02, 1230006. | 0.6 | 8 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6419 | Bridging Static and Dynamical Descriptions of Chemical Reactions: An <i>ab Initio</i> Study of CO ₂ Interacting with Water Molecules. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4029-4039. | 2.3 | 42 |
| 6420 | Errors in the Calculation of ²⁷ Al Nuclear Magnetic Resonance Chemical Shifts. <i>International Journal of Molecular Sciences</i> , 2012, 13, 15420-15446. | 1.8 | 9 |
| 6421 | Theoretical Prediction of the Complexation Behaviors of Antitumor Platinum Drugs with Cucurbiturils. <i>Journal of Physical Chemistry B</i> , 2012, 116, 14029-14039. | 1.2 | 42 |
| 6422 | Non-innocent ligand behaviour of a bimetallic Cu complex employing a bridging catecholate. <i>Dalton Transactions</i> , 2012, 41, 7905. | 1.6 | 13 |
| 6423 | Synthesis, characterisation and theoretical study of ruthenium 4,4'-bi-1,2,3-triazolyl complexes: fundamental switching of the nature of S1 and T1 states from MLCT to MC. <i>Dalton Transactions</i> , 2012, 41, 7637. | 1.6 | 47 |
| 6424 | Manganese K-Edge X-Ray Absorption Spectroscopy as a Probe of the Metal-Ligand Interactions in Coordination Compounds. <i>Inorganic Chemistry</i> , 2012, 51, 680-687. | 1.9 | 105 |
| 6425 | Size-Extensive Wave Functions for Quantum Monte Carlo: A Linear Scaling Generalized Valence Bond Approach. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1943-1951. | 2.3 | 35 |
| 6426 | Substituent Effects on the Thermochemistry of Thiophenes. A Theoretical (G3(MP2)//B3LYP and G3) Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4363-4370. | 1.1 | 6 |
| 6427 | <i>Ab initio</i> complex band structure of conjugated polymers: Effects of hybrid density functional theory and $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi mathvariant="italic"} \rangle \text{GW} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$ schemes. <i>Physical Review B</i> , 2012, 85, . | 1.1 | 34 |
| 6428 | Tuning of the Emission Efficiency and HOMO-LUMO Band Gap for Ester-Functionalized {Al(salophen)(H ₂ O) ₂ } ⁺ Blue Luminophors. <i>Inorganic Chemistry</i> , 2012, 51, 1309-1318. | 1.9 | 30 |
| 6429 | Structural and thermochemical properties of a photoresponsive spiropyran and merocyanine pair: Basis set and solvent dependence in density functional predictions. <i>Chemical Physics Letters</i> , 2012, 554, 60-66. | 1.2 | 19 |
| 6430 | Interplay of structural and electronic stabilizing factors in neutral and cationic phosphine protected Au ₁₃ clusters. <i>European Physical Journal D</i> , 2012, 66, 1. | 0.6 | 16 |
| 6431 | Mechanism of Lignin Dissolution and Regeneration in Ionic Liquid. <i>Energy & Fuels</i> , 2012, 26, 6393-6403. | 2.5 | 90 |
| 6432 | Water Adsorption at Two Unsolvated Peptides with a Protonated Lysine Residue: From Self-Solvation to Solvation. <i>Journal of Physical Chemistry B</i> , 2012, 116, 14788-14804. | 1.2 | 20 |
| 6433 | Spectroscopic Study on the Structural Differences of Thermally Induced Cross-Linking Segments in Emeraldine Salt and Base Forms of Polyaniline. <i>Journal of Physical Chemistry B</i> , 2012, 116, 14191-14200. | 1.2 | 24 |
| 6434 | Measuring the distance between two mercapto groups with an optical molecular ruler on the nanometer scale. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 15321. | 1.3 | 3 |
| 6435 | Initiators Based on Benzaldoximes: Bimolecular and Covalently Bound Systems. <i>Macromolecules</i> , 2012, 45, 8648-8657. | 2.2 | 16 |
| 6436 | Synthesis and study on oxidative coupling products of 3-alkyl-2-hydroxynaphthazarins. <i>Russian Chemical Bulletin</i> , 2012, 61, 2102-2108. | 0.4 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6437 | Conformational analysis of 2-acetylcyclopentanone by the density functional and MP2 methods. Russian Chemical Bulletin, 2012, 61, 2195-2203. | 0.4 | 1 |
| 6438 | Insights into the Charge Carrier Terahertz Mobility in Polyfluorenes from Large-Scale Atomistic Simulations and Time-Resolved Terahertz Spectroscopy. Journal of Physical Chemistry C, 2012, 116, 19665-19672. | 1.5 | 26 |
| 6440 | Microwave spectroscopy and quantum chemical investigation of nine low energy conformers of the 15-crown-5 ether. Physical Chemistry Chemical Physics, 2012, 14, 12912. | 1.3 | 15 |
| 6441 | Assigning Structures to Gas-Phase Peptide Cations and Cation-Radicals. An Infrared Multiphoton Dissociation, Ion Mobility, Electron Transfer, and Computational Study of a Histidine Peptide Ion. Journal of Physical Chemistry B, 2012, 116, 3445-3456. | 1.2 | 47 |
| 6442 | Ionic Conduction and Dielectric Response of Poly(imidazolium acrylate) Ionomers. Macromolecules, 2012, 45, 3974-3985. | 2.2 | 151 |
| 6443 | Tuning metal hydride thermodynamics via size and composition: Li ⁺ H, Mg ⁺ H, Al ⁺ H, and Mg ⁺ Al ⁺ H nanoclusters for hydrogen storage. Physical Chemistry Chemical Physics, 2012, 14, 6611. | 1.3 | 23 |
| 6444 | Charge Model 5: An Extension of Hirshfeld Population Analysis for the Accurate Description of Molecular Interactions in Gaseous and Condensed Phases. Journal of Chemical Theory and Computation, 2012, 8, 527-541. | 2.3 | 661 |
| 6445 | A new isomer of C ₂₀ and a way to a new C ₂₄₀ . Physical Chemistry Chemical Physics, 2012, 14, 14810. | 1.3 | 6 |
| 6446 | On the Computation of Adiabatic Energies in Aza-Boron-Dipyrromethene Dyes. Journal of Chemical Theory and Computation, 2012, 8, 3303-3313. | 2.3 | 102 |
| 6447 | QM/MM-Based Fitting of Atomic Polarizabilities for Use in Condensed-Phase Biomolecular Simulation. Journal of Chemical Theory and Computation, 2012, 8, 3839-3853. | 2.3 | 20 |
| 6448 | Complex Formation in Aqueous Trimethylamine- <i>N</i> -oxide (TMAO) Solutions. Journal of Physical Chemistry B, 2012, 116, 4783-4795. | 1.2 | 127 |
| 6449 | Mechanism of the Acid-Promoted Intramolecular Schmidt Reaction: Theoretical Assessment of the Importance of Lone Pair ⁺ Cation, Cation ⁺ π, and Steric Effects in Controlling Regioselectivity. Journal of Organic Chemistry, 2012, 77, 640-647. | 1.7 | 41 |
| 6450 | Structures and stabilities of group 17 fluorides EF ₃ (E = I, At, and element 117) with spin ⁺ orbit coupling. Physical Chemistry Chemical Physics, 2012, 14, 15816. | 1.3 | 18 |
| 6451 | Multi-decker tricarbonyl-bridged sandwich complexes of transition metals: structure, stability and electron-counting rules. Physical Chemistry Chemical Physics, 2012, 14, 14803. | 1.3 | 9 |
| 6452 | Explicitly correlated benchmark calculations on C ₈ H ₈ isomer energy separations: how accurate are DFT, double-hybrid, and composite <i>ab initio</i> procedures?. Molecular Physics, 2012, 110, 2477-2491. | 0.8 | 63 |
| 6453 | Improved semiconductor lattice parameters and band gaps from a middle-range screened hybrid exchange functional. Journal of Physics Condensed Matter, 2012, 24, 145504. | 0.7 | 72 |
| 6454 | Electronic Spectroscopy and Computational Studies of Glutathionylco(III)balamin. Journal of Physical Chemistry A, 2012, 116, 6851-6869. | 1.1 | 12 |
| 6455 | Molecular structure and bonding in octamethylporphyrin tin(II), SnN ₄ C ₂₈ H ₂₈ . Dalton Transactions, 2012, 41, 7550. | 1.6 | 23 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6456 | Lowest excited states and optical absorption spectra of donor-acceptor copolymers for organic photovoltaics: a new picture emerging from tuned long-range corrected density functionals. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14243. | 1.3 | 101 |
| 6457 | Mechanism of Atmospheric CO ₂ Fixation in the Cavities of a Dinuclear Cryptate. <i>Inorganic Chemistry</i> , 2012, 51, 5282-5288. | 1.9 | 23 |
| 6458 | Homogeneous Gold Catalysis: Hydration of 1,2-Diphenylacetylene with Methanol in Aqueous Media. A Theoretical Viewpoint. <i>Organometallics</i> , 2012, 31, 3074-3080. | 1.1 | 40 |
| 6459 | Computational Study on the Palladium-Catalyzed Allenylative Dearomatization Reaction. <i>Organometallics</i> , 2012, 31, 1168-1179. | 1.1 | 11 |
| 6460 | Quantum chemical studies on the enantiomerization mechanism of several [Zn(py) ₃ (tach)] ²⁺ derivatives. <i>Dalton Transactions</i> , 2012, 41, 14151. | 1.6 | 4 |
| 6461 | High-Level Ab Initio Predictions of the Energetics of $\text{CO}_2 \cdot \text{H}_2\text{O}$ ($n = 1, 2, 3$, $m = 1, 2$) Clusters. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9718-9729. | 1.1 | 14 |
| 6462 | Weak Antiferromagnetic Coupling via a Superexchange Interaction between Mn(II)-Mn(II) Ions: A QM/MM Study of the Active Site of Human Cytosolic X-Propyl Aminopeptidase P. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2293-2297. | 2.1 | 5 |
| 6464 | Thermal Conductivity of Graphene Nanoribbons: Effect of the Edges and Ribbon Width. <i>Journal of Heat Transfer</i> , 2012, 134, . | 1.2 | 4 |
| 6465 | QTAIM View of Metal-Metal Bonding in Di- and Trinuclear Disulfido Carbonyl Clusters. <i>Organometallics</i> , 2012, 31, 2559-2570. | 1.1 | 46 |
| 6466 | Thermodynamic and kinetic behaviour of [Pt(2-methylthiomethylpyridine)(OH ₂) ₂] ²⁺ . <i>Dalton Transactions</i> , 2012, 41, 512-522. | 1.6 | 24 |
| 6467 | Molecular Origins of Optoelectronic Properties in Coumarin Dyes: Toward Designer Solar Cell and Laser Applications. <i>Journal of Physical Chemistry A</i> , 2012, 116, 727-737. | 1.1 | 244 |
| 6468 | Engineering Tocopherol Selectivity in \hat{I}^{\pm} -TTP: A Combined In Vitro/In Silico Study. <i>PLoS ONE</i> , 2012, 7, e49195. | 1.1 | 10 |
| 6469 | THE INFRARED SPECTROSCOPY OF COMPACT POLYCYCLIC AROMATIC HYDROCARBONS CONTAINING UP TO 384 CARBONS. <i>Astrophysical Journal</i> , 2012, 754, 75. | 1.6 | 122 |
| 6470 | Silaphenolates and Silaphenylthiolates: Two Unexplored Unsaturated Silicon Compound Classes Influenced by Aromaticity. <i>Molecules</i> , 2012, 17, 369-389. | 1.7 | 6 |
| 6471 | Quantum Mechanics Calculations, Basicity and Crystal Structure: The Route to Transition Metal Complexes of Azahelicenes. <i>Molecules</i> , 2012, 17, 463-479. | 1.7 | 13 |
| 6472 | Density functional theory studies on structures and absorption spectra of [Au(tpy)Cl] ²⁺ and its derivatives: Role of basis set, functional, solvent effect, and spin orbit effect. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1642-1653. | 1.0 | 3 |
| 6473 | Relative stabilities of transition states determine diastereocontrol in sulfur ylide additions onto chiral α -sulfinyl imines. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 509-518. | 1.0 | 1 |
| 6474 | Performance of popular XC-functionals for the description of excitation energies in GFP-like chromophore models. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 789-800. | 1.0 | 51 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6475 | Kinetic parameters for the reaction of hydroxyl radical with CH ₃ OCH ₂ F (HFE-161) in the temperature range of 200–400 K: Transition state theory and Ab initio calculations. International Journal of Quantum Chemistry, 2012, 112, 1066-1077. | 1.0 | 12 |
| 6476 | Evaluation of DFT methods to study reactions of benzene with OH radical. International Journal of Quantum Chemistry, 2012, 112, 1879-1886. | 1.0 | 13 |
| 6477 | Reactions of ¹ S, ¹ D, and ³ P carbon atoms with water. Oxygen abstraction and intermolecular formaldehyde generation mechanisms; An MCSCF study. International Journal of Quantum Chemistry, 2012, 112, 1165-1184. | 1.0 | 10 |
| 6478 | Hydrogen bond and the resonance effect on the formamide–water complexes. International Journal of Quantum Chemistry, 2012, 112, 1401-1420. | 1.0 | 4 |
| 6479 | Interstitial water and the formation of low barrier hydrogen bonds: A computational model study. International Journal of Quantum Chemistry, 2012, 112, 1460-1472. | 1.0 | 2 |
| 6480 | Structure–Dependence of the magnetic moment in small palladium clusters: Surprising results from the M06–Meta–GGA functional. International Journal of Quantum Chemistry, 2012, 112, 113-120. | 1.0 | 10 |
| 6481 | Ni ₂ H and Ni ₂ Cl homolytic bond dissociation energies and radical stabilization energies: An assessment of theoretical procedures through comparison with benchmark-quality W2w data. International Journal of Quantum Chemistry, 2012, 112, 1862-1878. | 1.0 | 46 |
| 6482 | New Takes on Nitrate Ester Chemistry: Salts with Oxygen-Rich Ammonium Cations. Propellants, Explosives, Pyrotechnics, 2012, 37, 40-51. | 1.0 | 9 |
| 6483 | Linear free–energy relationships in semiquinone species and their Mn(II) and Cu(II) complexes. Journal of Physical Organic Chemistry, 2012, 25, 101-109. | 0.9 | 0 |
| 6484 | Spin–component–scaled electron correlation methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 886-906. | 6.2 | 197 |
| 6485 | Recent trends in conformational analysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 613-641. | 6.2 | 65 |
| 6486 | Syntheses, Crystal Structures and Thermal Behavior of Five New Complexes Containing 2, 4, 6–trifluorobenzoate as Ligand. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2012, 638, 1424-1431. | 0.6 | 14 |
| 6487 | Synthesis of and structure–property relationships in zinc complexes of bis–metaphenylene semiquinone biradical species. Journal of Physical Organic Chemistry, 2012, 25, 314-321. | 0.9 | 7 |
| 6488 | Synthesis and characterization of new derivatives of azulene, including experimental and theoretical studies of electronic and spectroscopic behavior. Journal of Physical Organic Chemistry, 2012, 25, 856-863. | 0.9 | 14 |
| 6489 | Reactions of substituted aspirins with amino acids. Journal of Physical Organic Chemistry, 2012, 25, 939-945. | 0.9 | 2 |
| 6490 | The nature of tryptophan radicals involved in the long–range electron transfer of lignin peroxidase and lignin peroxidase–like systems: Insights from quantum mechanical/molecular mechanics simulations. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1476-1483. | 1.5 | 17 |
| 6491 | DFT and <i>Ab Initio</i> calculations of spectroscopic properties of tetramethyltin and of its cation. International Journal of Quantum Chemistry, 2012, 112, 2032-2042. | 1.0 | 4 |
| 6492 | Electronic structure, dielectric properties and infrared vibrational spectrum of fayalite: An ab initio simulation with an all–electron Gaussian basis set and the B3LYP functional. International Journal of Quantum Chemistry, 2012, 112, 2098-2108. | 1.0 | 20 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6493 | Basis set and functional effects on excited-state properties: Three bicyclic chromogens as working examples. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2135-2141. | 1.0 | 36 |
| 6494 | Theoretical study of the chemical reactivity and molecular quantum similarity in a series of derivatives of 2- <i>adamantyl</i> -thiazolidine- <i>one</i> using density functional theory and the topological geometrical superposition approach. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2681-2687. | 1.0 | 17 |
| 6495 | Hydrogen-bonded complexes of nicotine with simple alcohols. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2787-2793. | 1.0 | 8 |
| 6496 | Bond pseudorotation, Jahn-Teller, and pseudo-Jahn-Teller effects in the cyclopentadienyl cation and its pentahalogeno derivatives. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3277-3288. | 1.0 | 25 |
| 6497 | Computing redox potentials for dyes used in <i>type dye</i> -sensitized solar cells. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3763-3768. | 1.0 | 4 |
| 6498 | The role of ion-bound cluster formation in negative ion mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2012, 26, 1923-1933. | 0.7 | 11 |
| 6499 | Surface Acoustic Wave Nebulization Produces Ions with Lower Internal Energy than Electrospray Ionization. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 1062-1070. | 1.2 | 53 |
| 6500 | Unveiling the Role of Molecule-Assisted Homolysis: A Mechanistic Probe into the Chemistry of a Bicyclic Peroxide. <i>Journal of Organic Chemistry</i> , 2012, 77, 2134-2141. | 1.7 | 4 |
| 6501 | Effects of curcumin and related compounds on processes involving $\dot{\text{I}}\pm$ -hydroxyethyl radicals. <i>Free Radical Research</i> , 2012, 46, 295-302. | 1.5 | 18 |
| 6502 | Computational Studies on Ethylene Addition to Nickel Bis(dithiolene). <i>Journal of Physical Chemistry A</i> , 2012, 116, 476-482. | 1.1 | 37 |
| 6503 | Regulation of NH-tautomerism in N-confused porphyrin by N-alkylation. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 4367. | 1.5 | 15 |
| 6504 | Excitation Gaps of Finite-Sized Systems from Optimally Tuned Range-Separated Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1515-1531. | 2.3 | 765 |
| 6505 | Halogen Bonding in DNA Base Pairs. <i>Journal of the American Chemical Society</i> , 2012, 134, 5165-5172. | 6.6 | 108 |
| 6506 | Heavy Atom Free Singlet Oxygen Generation: Doubly Substituted Configurations Dominate S_{11} States of Bis-BODIPYs. <i>Journal of Organic Chemistry</i> , 2012, 77, 4516-4527. | 1.7 | 117 |
| 6507 | Thermal stability of (MgO) ₁₂ dimers. <i>European Physical Journal D</i> , 2012, 66, 1. | 0.6 | 1 |
| 6508 | Planar P ₆ E ₆ (E = Se, S) macrocycles incorporating P ₂ N ₂ scaffolds. <i>Chemical Communications</i> , 2012, 48, 6346. | 2.2 | 43 |
| 6509 | Synthesis, IR-, NMR-, DFT- and X-ray analysis of novel C ₂ -chiral diferrocenyl-salen complexes. <i>Journal of Organometallic Chemistry</i> , 2012, 706-707, 46-51. | 0.8 | 4 |
| 6510 | Conformationally flexible chiral supramolecular catalysts for enantioselective Diels-Alder reactions with anomalous endo/exo selectivities. <i>Chemical Communications</i> , 2012, 48, 4273. | 2.2 | 63 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 6511 | σ-Back Donation from the Aromatic N-Substituent of N-Heterocyclic Carbene Ligands to Metal and Its Role in Catalysis. <i>Journal of the American Chemical Society</i> , 2012, 134, 8127-8135. | 6.6 | 60 |
| 6512 | Theoretical and experimental investigation on the electronic properties of the shuttlecock shaped and the double-decker structured metal phthalocyanines, MPc and M(Pc) ₂ (M = Sn and Pb). <i>Dalton Transactions</i> , 2012, 41, 7141. | 1.6 | 14 |
| 6513 | Gaseous Vanadium Molybdate and Tungstates: Thermodynamic Properties and Structures. <i>Inorganic Chemistry</i> , 2012, 51, 4918-4924. | 1.9 | 15 |
| 6514 | Strength of hydrogen bonds of water depends on local environment. <i>Journal of Chemical Physics</i> , 2012, 136, 144305. | 1.2 | 73 |
| 6515 | Challenges for Density Functional Theory. <i>Chemical Reviews</i> , 2012, 112, 289-320. | 23.0 | 1,869 |
| 6516 | Proton relay and electron flow in the O-O single bond formation in water oxidation by the ruthenium blue dimer. <i>Energy and Environmental Science</i> , 2012, 5, 7741. | 15.6 | 16 |
| 6517 | Fluoreno[4,3-c<i>f</i>]fluorene: A Closed-Shell, Fully Conjugated Hydrocarbon. <i>Organic Letters</i> , 2012, 14, 2426-2429. | 2.4 | 63 |
| 6518 | Vibrational Spectroscopic Studies of Molecules with Biochemical Interest: The Cysteine Zwitterion. <i>Applied Spectroscopy Reviews</i> , 2012, 47, 415-483. | 3.4 | 10 |
| 6519 | Application of the Multi-standard Methodology for Calculating ¹ H NMR Chemical Shifts. <i>Journal of Organic Chemistry</i> , 2012, 77, 6059-6065. | 1.7 | 83 |
| 6520 | Performance of the M11 and M11-L density functionals for calculations of electronic excitation energies by adiabatic time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11363. | 1.3 | 154 |
| 6521 | Chapter 2. Transition Metal Systems. <i>RSC Drug Discovery Series</i> , 2012, , 27-55. | 0.2 | 2 |
| 6522 | Bonds or not bonds? Pancake bonding in 1,2,3,5-dithiadiazolyl and 1,2,3,5-diselenadiazolyl radical dimers and their derivatives. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10713. | 1.3 | 72 |
| 6523 | Recent Advances in Wave Function-Based Methods of Molecular-Property Calculations. <i>Chemical Reviews</i> , 2012, 112, 543-631. | 23.0 | 549 |
| 6524 | The Role of Weak Bonding in Determining the Structure of Thiophene Oligomers inside Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9681-9690. | 1.5 | 26 |
| 6525 | Friedel-Crafts Acylation with Amides. <i>Journal of Organic Chemistry</i> , 2012, 77, 5788-5793. | 1.7 | 42 |
| 6526 | Modulation of energy levels by donor groups: an effective approach for optimizing the efficiency of zinc-porphyrin based solar cells. <i>Journal of Materials Chemistry</i> , 2012, 22, 7434. | 6.7 | 70 |
| 6527 | The Boron conundrum: the case of cationic clusters B _n ⁺ with n=2-20. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1. | 0.5 | 61 |
| 6528 | Electron-Deficiency Aromaticity in Silicon Nanoclusters. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2088-2094. | 2.3 | 20 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6529 | Donor-acceptor Copolymers of Relevance for Organic Photovoltaics: A Theoretical Investigation of the Impact of Chemical Structure Modifications on the Electronic and Optical Properties. <i>Macromolecules</i> , 2012, 45, 6405-6414. | 2.2 | 203 |
| 6530 | Benchmarking the performance of time-dependent density functional methods. <i>Journal of Chemical Physics</i> , 2012, 136, 104101. | 1.2 | 295 |
| 6531 | Dyotropic Rearrangements of Fused Tricyclic β -Lactones: Application to the Synthesis of (β)-Curcumanolide A and (β)-Curcumalactone. <i>Journal of the American Chemical Society</i> , 2012, 134, 13348-13356. | 6.6 | 74 |
| 6532 | The DFT investigations of the electron injection in hydrazone-based sensitizers. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1. | 0.5 | 49 |
| 6533 | DCMB that combines divide-and-conquer and mixed-basis set methods for accurate geometry optimizations, total energies, and vibrational frequencies of large molecules. <i>Journal of Computational Chemistry</i> , 2012, 33, 1421-1432. | 1.5 | 4 |
| 6534 | ERKALE—A flexible program package for X-ray properties of atoms and molecules. <i>Journal of Computational Chemistry</i> , 2012, 33, 1572-1585. | 1.5 | 70 |
| 6535 | Force field development for cofactors in the photosystem II. <i>Journal of Computational Chemistry</i> , 2012, 33, 1969-1980. | 1.5 | 53 |
| 6536 | An electronic structure theory investigation of the physical chemistry of the intermolecular complexes of cyclopropenylidene with hydrogen halides. <i>Journal of Computational Chemistry</i> , 2012, 33, 2073-2082. | 1.5 | 11 |
| 6537 | The role of the basis set and the level of quantum mechanical theory in the prediction of the structure and reactivity of cisplatin. <i>Journal of Computational Chemistry</i> , 2012, 33, 2292-2302. | 1.5 | 39 |
| 6538 | A new massively parallel version of CRYSTAL for large systems on high performance computing architectures. <i>Journal of Computational Chemistry</i> , 2012, 33, 2276-2284. | 1.5 | 43 |
| 6539 | Theoretical Study on the Gas-Phase S_N2 Reaction of Microhydrated Fluoride with Methyl Fluoride. <i>Journal of the Chinese Chemical Society</i> , 2012, 59, 1401-1408. | 0.8 | 6 |
| 6540 | Fragmentation of oxime and silyl oxime ether odd-electron positive ions by the McLafferty rearrangement: new insights on structural factors that promote β , γ fragmentation. <i>Journal of Mass Spectrometry</i> , 2012, 47, 676-686. | 0.7 | 11 |
| 6541 | Functionalization of gold and silver nanoparticles with diphenyl dichalcogenides probed by surface enhanced Raman scattering. <i>Journal of Raman Spectroscopy</i> , 2012, 43, 712-717. | 1.2 | 12 |
| 6542 | Density functional theory study of ^{13}C NMR chemical shift of chlorinated compounds. <i>Magnetic Resonance in Chemistry</i> , 2012, 50, 106-113. | 1.1 | 10 |
| 6543 | Structure and NMR spectra of cyclophanes with unsaturated bridges (cyclophanes). <i>Magnetic Resonance in Chemistry</i> , 2012, 50, 449-457. | 1.1 | 4 |
| 6544 | Structural and DFT Studies of Dibromine and Diiodine Adducts of a Sulfur-Rich Thiocarbonyl Donor. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 2373-2380. | 1.0 | 11 |
| 6545 | Catalytic Hydrocarbon Functionalization with Gold Complexes Containing N-Heterocyclic Carbene Ligands with Pendant Donor Groups. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 1380-1386. | 1.0 | 32 |
| 6546 | Cryptate Complexes with the Potential for CO_2 Activation: Quantum Chemical Predictions and Synthetic Efforts. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 4020-4028. | 1.0 | 5 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6547 | 2-Halogeno-1,3,2-diselenaphospholanes with an Annelated Dicarba-closo-dodecaborane(12) Unit: Synthesis, Molecular Structure and Reactivity. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 2908-2915. | 1.0 | 11 |
| 6548 | A Combined Experimental and Computational Study of the Magnetic Superexchange within a Triangular (1/3-O)-Pyrazolato-Fell3 Complex. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 3500-3506. | 1.0 | 15 |
| 6549 | Selective Consecutive Insertion of Alkynes into the B-Se Bonds of 1,3,2-Diselenaborolane Derivatives: Synthesis and Molecular Structures of Nine-Membered Rings. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 3909-3922. | 1.0 | 8 |
| 6550 | Mechanistic Insight into the Nickel-Catalyzed Intermolecular [3+2+2] Cycloaddition of Ethyl Cyclopropylideneacetate with Alkynes: DFT Calculations. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 3911-3915. | 1.2 | 13 |
| 6551 | Accurate Computation of Structures and Strain Energies of Cyclophanes with Modern DFT Methods. <i>Israel Journal of Chemistry</i> , 2012, 52, 180-192. | 1.0 | 38 |
| 6552 | Thermodynamics of chemical reactions with COSMO-RS: The extreme case of charge separation or recombination. <i>Journal of Computational Chemistry</i> , 2012, 33, 1304-1320. | 1.5 | 25 |
| 6553 | Assessment of <i>ab initio</i> MP2 and density functionals for characterizing the potential energy profiles of the S_N2 reactions at N center. <i>Journal of Computational Chemistry</i> , 2012, 33, 1347-1352. | 1.5 | 13 |
| 6554 | First Principles Design of Ionomers for Facile Ion Transport. <i>ACS Symposium Series</i> , 2012, , 19-44. | 0.5 | 6 |
| 6555 | Effects of Fluorination on Iridium(III) Complex Phosphorescence: Magnetic Circular Dichroism and Relativistic Time-Dependent Density Functional Theory. <i>Inorganic Chemistry</i> , 2012, 51, 2821-2831. | 1.9 | 48 |
| 6556 | Toward Accurate Theoretical Thermochemistry of First Row Transition Metal Complexes. <i>Journal of Physical Chemistry A</i> , 2012, 116, 870-885. | 1.1 | 138 |
| 6557 | Tuned Range-Separated Time-Dependent Density Functional Theory Applied to Optical Rotation. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 245-256. | 2.3 | 109 |
| 6558 | Tetrakis(diisopropyl amide) substituted norbornadiene and quadricyclane are highly barium selective ligands. <i>Dalton Transactions</i> , 2012, 41, 7037. | 1.6 | 5 |
| 6559 | Factors influencing Al ³⁺ -dimer speciation and stability from density functional theory calculations. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8058. | 1.3 | 18 |
| 6560 | Quantum Mechanical/Molecular Mechanical Study on the Mechanism of the Enzymatic Baeyer-Villiger Reaction. <i>Journal of the American Chemical Society</i> , 2012, 134, 2732-2741. | 6.6 | 90 |
| 6561 | Mixed-Valence Nickel-Iron Dithiolate Models of the [NiFe]-Hydrogenase Active Site. <i>Inorganic Chemistry</i> , 2012, 51, 2338-2348. | 1.9 | 67 |
| 6562 | Electron transfer beyond the static picture: A TDDFT/TD-ZINDO study of a pentacene dimer. <i>Journal of Chemical Physics</i> , 2012, 137, 22A502. | 1.2 | 11 |
| 6563 | Bistriphenylamine-based organic sensitizers with high molar extinction coefficients for dye-sensitized solar cells. <i>RSC Advances</i> , 2012, 2, 6209. | 1.7 | 18 |
| 6564 | Significant Improvement of Dye-Sensitized Solar Cell Performance by Small Structural Modification in π -Conjugated Donor-Acceptor Dyes. <i>Advanced Functional Materials</i> , 2012, 22, 1291-1302. | 7.8 | 404 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6569 | Highly Enantioselective Synthesis of 3-Substituted Furanones by Palladium-Catalyzed Kinetic Resolution of Unsymmetrical Allyl Acetates. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 3168-3173. | 7.2 | 57 |
| 6570 | A Combined Gas-Phase Photoelectron Spectroscopic and Theoretical Study of Zeise's Anion and Its Bromine and Iodine Analogues. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 6356-6360. | 7.2 | 11 |
| 6571 | Synthesis, characterization, biological studies and <i>in vitro</i> cytotoxicity on human cancer cell lines of titanium(IV) and tin(IV) derivatives with the 1,1'-bis(2-mercapto-2-oxoethyl)ethylene ligand. <i>Applied Organometallic Chemistry</i> , 2012, 26, 383-389. | 1.7 | 7 |
| 6572 | The Catalytic Potential of Substituted Pyridines in Acylation Reactions: Theoretical Prediction and Experimental Validation. <i>ChemCatChem</i> , 2012, 4, 559-566. | 1.8 | 16 |
| 6573 | Low-Temperature CO Oxidation over Cu-Based Metal-Organic Frameworks Monitored by using FTIR Spectroscopy. <i>ChemCatChem</i> , 2012, 4, 755-759. | 1.8 | 38 |
| 6574 | Dihydrogen Generation from Amine/Boranes: Synthesis, FT-IR, and Computational Studies. <i>Chemistry - A European Journal</i> , 2012, 18, 3981-3991. | 1.7 | 38 |
| 6575 | Highly Efficient Redox Isomerisation of Allylic Alcohols Catalysed by Pyrazole-Based Ruthenium(IV) Complexes in Water: Mechanisms of Bifunctional Catalysis in Water. <i>Chemistry - A European Journal</i> , 2012, 18, 7749-7765. | 1.7 | 68 |
| 6576 | Molecular Tethering or Aggregation: Is the Existence of Charge-Transfer Bands Indicative of the Formation of Blue-Box/Tetrathiafulvalene Inclusion Complexes?. <i>Chemistry - A European Journal</i> , 2012, 18, 5606-5611. | 1.7 | 14 |
| 6577 | Silicon-Containing Formal 4i-Electron Four-Membered Ring Systems: Antiaromatic, Aromatic, or Nonaromatic?. <i>Chemistry - A European Journal</i> , 2012, 18, 7516-7524. | 1.7 | 51 |
| 6578 | Total Synthesis of Exiguamines A and B Inspired by Catecholamine Chemistry. <i>Chemistry - A European Journal</i> , 2012, 18, 4999-5005. | 1.7 | 34 |
| 6579 | Correspondence of Ru ^{III} and Ru ^{II} and Ru ^{IV} Ru ^{III} Mixed Valent States in a Small Dinuclear Complex. <i>Chemistry - A European Journal</i> , 2012, 18, 5667-5675. | 1.7 | 29 |
| 6580 | An Experimental Study on the Effect of Substituents on Aromatic-Aromatic Interactions in Dithia[3,3]metaparacyclophanes. <i>Chemistry - A European Journal</i> , 2012, 18, 3611-3620. | 1.7 | 29 |
| 6581 | Bifunctional Rhenium Complexes for the Catalytic Transfer-Hydrogenation Reactions of Ketones and Imines. <i>Chemistry - A European Journal</i> , 2012, 18, 5701-5714. | 1.7 | 40 |
| 6582 | A Mechanistic Study of the Utilization of <i>arachno</i> Diruthenaborane [(Cp* ₂ RuCO) ₂ B ₂ H ₆] as an Active Alkyne-Cyclotrimerization Catalyst. <i>Chemistry - A European Journal</i> , 2012, 18, 8482-8489. | 1.7 | 55 |
| 6583 | Gutmann Donor and Acceptor Numbers for Ionic Liquids. <i>Chemistry - A European Journal</i> , 2012, 18, 10969-10982. | 1.7 | 168 |
| 6584 | Expanding the Horizon of the Thymine Isostere Biochemistry: Unique Cyclobutane Dimers Formed by Photoreaction between a Thymine and a Toluene Residue in the Dinucleotide Framework. <i>Chemistry - A European Journal</i> , 2012, 18, 7823-7833. | 1.7 | 6 |
| 6585 | Mechanism of Silver(I)-Catalyzed Enantioselective Synthesis of Axially Chiral Allenes Based on Propargylamines. <i>Chinese Journal of Chemistry</i> , 2012, 30, 951-958. | 2.6 | 18 |
| 6586 | Spin-Spin Artificial DNA Intercalated with Silver Cations: Theoretical Prediction. <i>ChemPhysChem</i> , 2012, 13, 1332-1338. | 1.0 | 8 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6587 | Gas-Phase Thermodynamics as a Validation of Computational Catalysis on Surfaces: A Case Study of Fischer-Tropsch Synthesis. <i>ChemPhysChem</i> , 2012, 13, 1486-1494. | 1.0 | 23 |
| 6588 | Conformations of Serine in Aqueous Solutions as Revealed by Vibrational Circular Dichroism. <i>ChemPhysChem</i> , 2012, 13, 1272-1281. | 1.0 | 41 |
| 6589 | B ₃ N ₃ Borazine Substitution in Hexa-peri-Hexabenzocoronene: Computational Analysis and Scholl Reaction of Hexaphenylborazine. <i>ChemPhysChem</i> , 2012, 13, 1173-1181. | 1.0 | 47 |
| 6590 | Single-Crystal X-Ray Diffraction, Isolated Molecule and Cluster Electronic Structure Calculations, and Scanning Electron Microscopy in an Organic solid: Models for Intramolecular Motion in 4,4'-Dimethoxybiphenyl. <i>ChemPhysChem</i> , 2012, 13, 2082-2089. | 1.0 | 12 |
| 6591 | Conformational Distributions of N-Acetyl-L-cysteine in Aqueous Solutions: A Combined Implicit and Explicit Solvation Treatment of VA and VCD Spectra. <i>ChemPhysChem</i> , 2012, 13, 2310-2321. | 1.0 | 41 |
| 6592 | Structural Characteristics of Graphene-Type C and BN Nanostructures by Periodic Local MP2 Approach. <i>ChemPhysChem</i> , 2012, 13, 2361-2367. | 1.0 | 9 |
| 6593 | Aggregation and Solvation of Chiral N-Amide Ligands in Coordinating Solvents: A Computational and NMR Spectroscopic Study. <i>ChemPlusChem</i> , 2012, 77, 799-806. | 1.3 | 11 |
| 6594 | Atomic Layer Deposition of Tantalum Oxide and Tantalum Silicate from Chloride Precursors. <i>Chemical Vapor Deposition</i> , 2012, 18, 225-238. | 1.4 | 14 |
| 6595 | Vibrational Davydov Splittings and Collective Mode Polarizations in Oriented Organic Semiconductor Crystals. <i>Journal of Physical Chemistry C</i> , 2012, 116, 14491-14503. | 1.5 | 25 |
| 6596 | Hybrid QM/MM Molecular Dynamics Study of Benzocaine in a Membrane Environment: How Does a Quantum Mechanical Treatment of Both Anesthetic and Lipids Affect Their Interaction. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2197-2203. | 2.3 | 20 |
| 6597 | Assessment of density functional theory to calculate the phase transition pressure of ice. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11484. | 1.3 | 22 |
| 6598 | Substituent Effects in Thermal Reactions of a Silene with Silyl-Substituted Alkynes: A Theoretical Study. <i>Organometallics</i> , 2012, 31, 4737-4747. | 1.1 | 7 |
| 6599 | Endohedral Beryllium Atoms in Germanium Clusters with Eight and Fewer Vertices: How Small Can a Cluster Be and Still Encapsulate a Central Atom?. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5227-5234. | 1.1 | 7 |
| 6600 | Supramolecular interactions between hexabromoethane and cyclopentadienyl ruthenium bromides: Halogen bonding or electrostatic organisation?. <i>CrystEngComm</i> , 2012, 14, 804-811. | 1.3 | 19 |
| 6601 | Photophysical and electrochemical properties of 1,3-bis(2-pyridylimino)isoindolate platinum(ii) derivatives. <i>Dalton Transactions</i> , 2012, 41, 8648. | 1.6 | 19 |
| 6602 | Performance assessment of density functional theory-based models using orbital momentum distributions. <i>Molecular Simulation</i> , 2012, 38, 468-480. | 0.9 | 4 |
| 6603 | Ruthenium(ii) [3 + 2 + 1] mixed ligand complexes: substituent effect on photolability, photooxidation of bases, photocytotoxicity and photonuclease activity. <i>Dalton Transactions</i> , 2012, 41, 8460. | 1.6 | 17 |
| 6604 | Communication: Density functional theory overcomes the failure of predicting intermolecular interaction energies. <i>Journal of Chemical Physics</i> , 2012, 136, 161102. | 1.2 | 68 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6605 | Anion-Directed Formation and Degradation of an Interlocked Metallohelicate. <i>Journal of the American Chemical Society</i> , 2012, 134, 10987-10997. | 6.6 | 116 |
| 6606 | Effect of Axial Ligand on the Electronic Configuration, Spin States, and Reactivity of Iron Oxophlorin. <i>Inorganic Chemistry</i> , 2012, 51, 7094-7102. | 1.9 | 17 |
| 6607 | Mechanistic study on the palladium-catalyzed (3 + 2) intramolecular cycloaddition of alk-5-enylidene cyclopropanes. <i>Dalton Transactions</i> , 2012, 41, 9468. | 1.6 | 21 |
| 6608 | The effect of hydrogen bonding on the excited-state proton transfer in 2-(2-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 9016. | 1.3 | 69 |
| 6609 | Hypervalent Sulfur-Functionalized Diphosphagermylene and Diphosphastannylene Compounds. <i>Organometallics</i> , 2012, 31, 246-255. | 1.1 | 14 |
| 6610 | Copper(II)-Binding Ability of Stereoisomeric <i>cis</i> - and <i>trans</i> -2-Aminocyclohexanecarboxylic Acid- <i>l</i> -Phenylalanine Dipeptides. A Combined CW/Pulsed EPR and DFT Study. <i>Inorganic Chemistry</i> , 2012, 51, 1386-1399. | 1.9 | 21 |
| 6611 | Platinated DNA Affects Zinc Finger Conformation. Interaction of a Platinated Single-Stranded Oligonucleotide and the C-Terminal Zinc Finger of Nucleocapsid Protein HIVNCp7. <i>Biochemistry</i> , 2012, 51, 1752-1761. | 1.2 | 19 |
| 6612 | Accurate thermochemistry from a parameterized coupled-cluster singles and doubles model and a local pair natural orbital based implementation for applications to larger systems. <i>Journal of Chemical Physics</i> , 2012, 136, 064101. | 1.2 | 68 |
| 6613 | Combined experimental and theoretical studies on the photophysical properties of cycloparaphenylenes. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 5979. | 1.5 | 248 |
| 6614 | Advances in ab-initio theory of multiferroics. <i>European Physical Journal B</i> , 2012, 85, 1. | 0.6 | 35 |
| 6615 | Tunable Charge Tags for Electron-Based Methods of Peptide Sequencing: Design and Applications. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 608-620. | 1.2 | 14 |
| 6616 | A Negative Ion Mass Spectrometry Approach to Identify Cross-Linked Peptides Utilizing Characteristic Disulfide Fragmentations. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 1364-1375. | 1.2 | 15 |
| 6617 | Cascade Dissociations of Peptide Cation-Radicals. Part 2. Infrared Multiphoton Dissociation and Mechanistic Studies of <i>b</i> - and <i>y</i> -Ions from Pentapeptides. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 1351-1363. | 1.2 | 28 |
| 6618 | Structure of the complex UCl ₄ ·2DMF by vibrational infrared spectroscopy and density functional theory. <i>Journal of Applied Spectroscopy</i> , 2012, 79, 22-30. | 0.3 | 6 |
| 6619 | Structure and vibrational IR spectra of a UCl ₄ ·2DMSO complex. <i>Journal of Applied Spectroscopy</i> , 2012, 79, 165-172. | 0.3 | 5 |
| 6620 | Synthesis and Characterization of 5-Amino-1-nitriminotetrazole and Its Salts. <i>Journal of Chemical Crystallography</i> , 2012, 42, 816-823. | 0.5 | 12 |
| 6621 | X-Ray Diffraction and Theoretical Approach to the Molecular Structure of (E)-2-(2-(1,3-dioxisoindolin-2-yl)-1-(3-phenyl-3-methylcyclobutyl)ethylidene) hydrazine carboxamide. <i>Journal of Chemical Crystallography</i> , 2012, 42, 897-904. | 0.5 | 10 |
| 6622 | Conformational analysis of caprolactam, cycloheptene and caprolactone. <i>Structural Chemistry</i> , 2012, 23, 723-732. | 1.0 | 20 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6623 | A combined experimental and DFT study on the complexation of Mg ²⁺ with beauvericin. Structural Chemistry, 2012, 23, 765-769. | 1.0 | 3 |
| 6624 | EL: the new aromaticity measure based on one-electron density function. Structural Chemistry, 2012, 23, 1173-1183. | 1.0 | 42 |
| 6625 | Control of ionic properties of N-nitrosodimethylamine through hydrogen substitution by fluorine atoms. Structural Chemistry, 2012, 23, 1193-1201. | 1.0 | 2 |
| 6626 | Energetics of dioxygen binding into graphene patches with various sizes and shapes. Science China Chemistry, 2012, 55, 787-795. | 4.2 | 2 |
| 6627 | CH ₂ , NH, and O heteroatom substitution effects on the electronic, optical, and charge transport properties of a 2,1,3-benzothiadiazole-based derivative: Insights from theory. Science China Chemistry, 2012, 55, 1364-1369. | 4.2 | 2 |
| 6628 | Computational ¹⁹ F NMR. 1. General features. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 19 |
| 6629 | The nature of the C≡As bonds in arsaalkynes: an atoms in molecules and electron localization function study. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 8 |
| 6630 | On the kinetics and thermodynamics of S-X (X=H, CH ₃ , SCH ₃ , COCH ₃ , and CN) cleavage in the formation of self-assembled monolayers of alkylthiols on Au(111). Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 17 |
| 6631 | Optimization of the explicit polarization (X-Pol) potential using a hybrid density functional. Theoretical Chemistry Accounts, 2012, 131, 1161. | 0.5 | 15 |
| 6632 | [Zn ₁₀ (μ ₄ -S)(μ ₃ -S) ₆ (Py) ₉ (SO ₄) ₃] as a molecular model of ZnS surfaces: an experimental and theoretical study. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 0 |
| 6633 | Adsorption of successive layers of H ₂ molecules on a model copper surface: performances of second- to fifth-rung exchange-correlation functionals. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 3 |
| 6634 | The sphericity of the diverse 10-vertex polyhedra found in bare post-transition metal clusters: germanium clusters with interstitial magnesium atoms as model systems. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 2 |
| 6635 | Quantum chemical study of self-doping PPV oligomers: spin distribution of the radical forms. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 4 |
| 6636 | A systematical comparison of DFT methods in reproducing the interaction energies of halide series with protein moieties. Journal of Molecular Modeling, 2012, 18, 2079-2098. | 0.8 | 6 |
| 6637 | Ab initio and DFT study of luminescent cyclometalated N-heterocyclic carbene organogold(III) complexes. Journal of Molecular Modeling, 2012, 18, 2543-2551. | 0.8 | 4 |
| 6638 | Estimating the carbonyl anharmonic vibrational frequency from affordable harmonic frequency calculations. Journal of Molecular Modeling, 2012, 18, 2471-2478. | 0.8 | 10 |
| 6639 | A comparative study on the B ₁₂ N ₁₂ , Al ₁₂ N ₁₂ , B ₁₂ P ₁₂ and Al ₁₂ P ₁₂ fullerene-like cages. Journal of Molecular Modeling, 2012, 18, 2653-2658. | 0.8 | 160 |
| 6640 | Computational study of the Sonogashira cross-coupling reaction in the gas phase and in dichloromethane solution. Journal of Molecular Modeling, 2012, 18, 3025-3033. | 0.8 | 16 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6641 | On the potential application of DFT methods in predicting the interaction-induced electric properties of molecular complexes. Molecular H-bonded chains as a case of study. <i>Journal of Molecular Modeling</i> , 2012, 18, 3073-3086. | 0.8 | 29 |
| 6642 | First- and second-row transition metal oxa-aza macrocyclic complexes: a DFT study of an octahedral conformation. <i>Journal of Molecular Modeling</i> , 2012, 18, 3243-3253. | 0.8 | 8 |
| 6643 | Efficient nucleation of stardust silicates via heteromolecular homogeneous condensation. <i>Monthly Notices of the Royal Astronomical Society</i> , 2012, , no-no. | 1.6 | 33 |
| 6644 | Structural analysis of methyl 6-O-benzyl-2-deoxy-2-dimethylmaleimido- β -D-allopyranoside by X-ray crystallography, NMR, and QM calculations: hydrogen bonding and comparison of density functionals. <i>Carbohydrate Research</i> , 2012, 353, 79-85. | 1.1 | 3 |
| 6645 | Essential role of glutamate 317 in galactosyl transfer by β 3GalT: a computational study. <i>Carbohydrate Research</i> , 2012, 356, 204-208. | 1.1 | 17 |
| 6646 | Can water be a catalyst on the HO ₂ +H ₂ O+O ₃ reactive cluster?. <i>Chemical Physics</i> , 2012, 399, 17-22. | 0.9 | 19 |
| 6647 | Theoretical modelling of the adsorption of thallium and element 113 atoms on gold using two-component density functional methods with effective core potentials. <i>Chemical Physics</i> , 2012, 395, 95-103. | 0.9 | 22 |
| 6648 | The azido oxide N ₃ O. <i>Chemical Physics</i> , 2012, 398, 129-133. | 0.9 | 0 |
| 6649 | Nuclear size effects in rotational spectra: A tale with a twist. <i>Chemical Physics</i> , 2012, 401, 103-112. | 0.9 | 14 |
| 6650 | A benchmark test suite for proton transfer energies and its use to test electronic structure model chemistries. <i>Chemical Physics</i> , 2012, 400, 8-12. | 0.9 | 36 |
| 6651 | Stereochemical characterization of fluorinated 2-(phenanthren-1-yl)propionic acids by enantioselective high performance liquid chromatography analysis and electronic circular dichroism detection. <i>Journal of Chromatography A</i> , 2012, 1232, 128-133. | 1.8 | 4 |
| 6652 | Separation of unsaturated organic compounds using silver ⁺ thiolate chromatographic material. <i>Journal of Chromatography A</i> , 2012, 1240, 83-89. | 1.8 | 41 |
| 6653 | The unimolecular thermal decomposition mechanism of syn, anti-N,N ² -Dinitrourea (DNU). <i>Combustion and Flame</i> , 2012, 159, 1393-1398. | 2.8 | 7 |
| 6654 | New range-separated hybrids based on the TCA density functional. <i>Chemical Physics Letters</i> , 2012, 519-520, 145-149. | 1.2 | 5 |
| 6655 | Constrained self-consistent field method revisited toward theoretical designs of functional materials under external field. <i>Chemical Physics Letters</i> , 2012, 530, 132-136. | 1.2 | 3 |
| 6656 | Decomposition mechanisms and dynamics of N ₆ : Bond orders and partial charges along classical trajectories. <i>Chemical Physics Letters</i> , 2012, 531, 46-51. | 1.2 | 25 |
| 6657 | A density functional theory study on the most stable ultra long B ⁺ N co-doped (5,5) single walled carbon nanotubes. <i>Chemical Physics Letters</i> , 2012, 532, 90-95. | 1.2 | 2 |
| 6658 | THz spectroscopic investigation of chlorotoluron by solid-state density functional theory. <i>Chemical Physics Letters</i> , 2012, 534, 72-76. | 1.2 | 10 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6659 | Seeking for reliable double-hybrid density functionals without fitting parameters: The PBE0-2 functional. <i>Chemical Physics Letters</i> , 2012, 538, 121-125. | 1.2 | 118 |
| 6660 | Synthesis and photophysical properties of covalently linked boron dipyrromethene dyads. <i>Dyes and Pigments</i> , 2012, 94, 66-73. | 2.0 | 21 |
| 6661 | Theoretical studies on structures and electronic spectra of linear HC _n N ⁺ (n=2-14). <i>International Journal of Mass Spectrometry</i> , 2012, 309, 56-62. | 0.7 | 4 |
| 6662 | Protonation sites in peptide dications and cation-radicals containing $\hat{1}^2$ -amino acid residues. <i>International Journal of Mass Spectrometry</i> , 2012, 316-318, 57-67. | 0.7 | 5 |
| 6663 | A theoretical elucidation of coordination properties of histidine and lysine to Mn ²⁺ . <i>International Journal of Mass Spectrometry</i> , 2012, 313, 47-57. | 0.7 | 10 |
| 6664 | Magnetic properties of single crystal alpha-benzoin oxime: An EPR study. <i>Radiation Physics and Chemistry</i> , 2012, 81, 146-151. | 1.4 | 10 |
| 6665 | Theoretical study of the addition and abstraction reactions of hydroxyl radical with uracil. <i>Radiation Physics and Chemistry</i> , 2012, 81, 267-272. | 1.4 | 32 |
| 6666 | Synthesis, spectroscopic characterizations and quantum chemical computational studies of (Z)-4-[(E)-(4-fluorophenyl)diazenyl]-6-[(3-hydroxypropylamino)methylene]-2-methoxycyclohexa-2,4-dienone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 85, 85-91. | 2.0 | 20 |
| 6667 | NMR, UV, FT-IR, FT-Raman spectra and molecular structure (monomeric and dimeric structures) investigation of nicotinic acid N-oxide: A combined experimental and theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 85, 145-154. | 2.0 | 56 |
| 6668 | Theoretical investigations of $\hat{1}^{\pm}, \hat{1}^{\pm}$ -trifluoro-3-, -p and -o-nitrotoluene by means of density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 85, 271-282. | 2.0 | 7 |
| 6669 | Synthesis, characterization and DFT study of methoxybenzylidene containing chromophores for DSSC materials. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 239-243. | 2.0 | 46 |
| 6670 | Theoretical and experimental study on the excited states of the X-, $\hat{1}^{\pm}$ - and $\hat{1}^2$ -forms of lithium phthalocyanine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 118-125. | 2.0 | 9 |
| 6671 | Synthesis, spectroscopic characterizations and quantum chemical computational studies of (Z)-4-[(E)-p-tolyldiazenyl]-6-[(2-hydroxyphenylamino)methylene]-2-methoxycyclohexa-2,4-dienone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 92, 357-364. | 2.0 | 38 |
| 6672 | A theoretical study on the molecular structure and vibrational (FT-IR and Raman) spectra of cyano-bridged heteronuclear polymeric complex of triethylenetetramine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 94, 110-118. | 2.0 | 14 |
| 6673 | Survey of conformational isomerism in (E)-2-[(4-bromophenylimino)methyl]-5-(diethylamino)phenol compound from structural and thermochemical points of view. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 95, 664-669. | 2.0 | 6 |
| 6674 | Experimental and theoretical investigation of the molecular and electronic structure of 3-ethoxy-4-isopropylaminocyclobut-3-ene-1,2-dione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 35-41. | 2.0 | 12 |
| 6675 | Spectroscopic, electronic structure and natural bond analysis of 2-aminopyrimidine and 4-aminopyrazolo[3,4-d]pyrimidine: A comparative study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 226-241. | 2.0 | 19 |
| 6676 | Theoretical infrared spectra of biphenyl, terphenyls and tetraphenyls for astrophysical purposes. <i>Journal of Molecular Spectroscopy</i> , 2012, 275, 21-27. | 0.4 | 6 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6677 | Vibronic fine-structure in the S ₀ →S ₁ absorption spectrum of zinc porphyrin: A Franck-Condon simulation incorporating Herzberg-Teller theory and the Duschinsky effect. <i>Journal of Molecular Spectroscopy</i> , 2012, 275, 61-70. | 0.4 | 13 |
| 6678 | Modeling of a violaxanthin-chlorophyll b chromophore pair in its LHCII environment using CAM-B3LYP. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2012, 109, 12-19. | 1.7 | 17 |
| 6679 | Effects of TiO ₂ nanoparticle polymorphism on dye-sensitized solar cell photovoltaic properties. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2012, 232, 22-31. | 2.0 | 71 |
| 6680 | Ab initio study of the silicon-bismuth interface: Bismuth nanolines and bismuth-covered silicon nanoparticles. <i>Microelectronic Engineering</i> , 2012, 90, 99-103. | 1.1 | 1 |
| 6681 | Effect of zirconium addition on vanadium-catalyzed toluene oxidation by H ₂ O ₂ in CH ₃ COOH. <i>Journal of Molecular Catalysis A</i> , 2012, 357, 1-10. | 4.8 | 21 |
| 6682 | Molecular structure, vibrational spectra, NBO analysis, first hyperpolarizability, and HOMO, LUMO studies of mesityl chloride by density functional methods. <i>Journal of Molecular Structure</i> , 2012, 1007, 136-145. | 1.8 | 33 |
| 6683 | Quantum chemical calculations and experimental investigations on 2-aminobenzoic acid-cyclodiphosph(V)azane derivative and its homo-binuclear Cu(II) complex. <i>Journal of Molecular Structure</i> , 2012, 1011, 50-58. | 1.8 | 10 |
| 6684 | Structure of 2,3-dicarboxy-1-methylpyridinium monohydrate studied by X-ray diffraction, DFT calculations, FTIR, Raman and NMR spectra. <i>Journal of Molecular Structure</i> , 2012, 1013, 1-10. | 1.8 | 6 |
| 6685 | Comparison of the performance of different DFT methods in the calculations of the molecular structure and vibration spectra of serotonin (5-hydroxytryptamine, 5-HT). <i>Journal of Molecular Structure</i> , 2012, 1013, 111-118. | 1.8 | 9 |
| 6686 | Structural and thermal behavior of imidazolium N,N'-dinitrourea. <i>Journal of Molecular Structure</i> , 2012, 1015, 67-73. | 1.8 | 7 |
| 6687 | Molecular design of new hydrazone dyes for dye-sensitized solar cells: Synthesis, characterization and DFT study. <i>Journal of Molecular Structure</i> , 2012, 1019, 130-134. | 1.8 | 39 |
| 6688 | Synthesis, structure and antimicrobial activity of 6-(propan-2-yl)-3-methyl-morpholine-2,5-dione. <i>Journal of Molecular Structure</i> , 2012, 1016, 147-154. | 1.8 | 14 |
| 6689 | Investigating the prototropic tautomerism in (E)-2-[(4-fluorophenyl)iminomethyl]-5-methoxyphenol compound for solid state and solvent media by experimental and quantum computational tools. <i>Journal of Molecular Structure</i> , 2012, 1017, 38-44. | 1.8 | 19 |
| 6690 | Polyamines V: The structure of tetramethylene-1,4-bis(N-deoxyglucitolammonium chloride) studied by X-ray diffraction, DFT calculations, NMR and FTIR spectroscopy. <i>Journal of Molecular Structure</i> , 2012, 1020, 41-47. | 1.8 | 3 |
| 6691 | Synthesis, experimental and theoretical study of the spectroscopic properties in (2E)-3-{3-methoxy-4-[(3-methylbut-2-en-1-yl)oxy]phenyl}-1-(3,4,5-trimethoxyphenyl)prop-2-en-1-one. <i>Journal of Molecular Structure</i> , 2012, 1020, 88-95. | 1.8 | 9 |
| 6692 | Synthesis, structural investigations, and DFT calculations on novel 3-(1,3-dioxan-2-yl)-10-methyl-10H-phenothiazine derivatives with fluorescence properties. <i>Tetrahedron</i> , 2012, 68, 2465-2470. | 1.0 | 16 |
| 6693 | Efficient sonochemical synthesis of alkyl 4-aryl-6-chloro-5-formyl-2-methyl-1,4-dihydropyridine-3-carboxylate derivatives. <i>Ultrasonics Sonochemistry</i> , 2012, 19, 221-226. | 3.8 | 17 |
| 6694 | Modification of the electric properties of molecular devices via gradual increase of number of nitrogen atoms: A computational study. <i>Organic Electronics</i> , 2012, 13, 807-814. | 1.4 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6695 | DFT studies on the reaction of CO ₂ with allyl-bridged dinuclear palladium(I) complexes. <i>Polyhedron</i> , 2012, 32, 35-40. | 1.0 | 27 |
| 6696 | Theoretical study of the structure and spectroscopic characterization of the new 1-ferrogermene in the gas phase. <i>Polyhedron</i> , 2012, 31, 29-36. | 1.0 | 6 |
| 6697 | Synthesis and characterization of 11-vertex platinaborane compounds having nido-PtB ₁₀ H ₁₂ and nido-Pt ₂ B ₉ H ₁₀ skeletons. <i>Polyhedron</i> , 2012, 31, 607-613. | 1.0 | 4 |
| 6698 | Effect of weak sulfurâ€¦C(â€¦) interactions, and hydrogen bonds in supramolecular association of chlorodiphenyltin(IV) dithiocarbamate complexes: Study of their stability in solution. <i>Polyhedron</i> , 2012, 33, 223-234. | 1.0 | 21 |
| 6699 | Kinetic versus thermodynamic isomers of the deltahedral dicobaltadecaboranes having nine to 12 vertices. <i>Polyhedron</i> , 2012, 33, 319-326. | 1.0 | 6 |
| 6700 | Effect of electron count on the structures of (benzene)metallaboranes with 9â€¦12 vertices: Comparison of the iron and ruthenium systems. <i>Polyhedron</i> , 2012, 40, 110-117. | 1.0 | 2 |
| 6701 | Analysis of indolylfulgide spectral properties using time dependent density functional theory. <i>Journal of Luminescence</i> , 2012, 132, 1929-1934. | 1.5 | 11 |
| 6702 | Binding of TNT to amplifying fluorescent polymers: An ab initio and molecular dynamics study. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 33, 12-18. | 1.3 | 12 |
| 6703 | Raman spectroscopy and DFT calculations of para-coumaric acid and its deprotonated species. <i>Vibrational Spectroscopy</i> , 2012, 58, 139-145. | 1.2 | 14 |
| 6704 | Experimental and Theoretical Studies on Organic Dâ€¦A Systems Containing Threeâ€¦Coordinate Boron Moieties as both â€¦Donor and â€¦Acceptor. <i>Chemistry - A European Journal</i> , 2012, 18, 1369-1382. | 1.7 | 80 |
| 6705 | Influential Role of Ethereal Solvent on Organolithium Compounds: The Case of Carboranylithium. <i>Chemistry - A European Journal</i> , 2012, 18, 3174-3184. | 1.7 | 50 |
| 6706 | Catalytic Nonâ€¦Conventional <i>trans</i> -â€¦Hydroboration: A Theoretical and Experimental Perspective. <i>Chemistry - A European Journal</i> , 2012, 18, 1512-1521. | 1.7 | 54 |
| 6707 | Quantum mechanically derived AMBERâ€¦compatible heme parameters for various states of the cytochrome P450 catalytic cycle. <i>Journal of Computational Chemistry</i> , 2012, 33, 119-133. | 1.5 | 210 |
| 6708 | Mechanism for the reaction of 2â€¦naphthol with <i>N,N</i> -methylâ€¦phenylâ€¦hydrazine suggested by the density functional theory investigations. <i>Journal of Computational Chemistry</i> , 2012, 33, 220-230. | 1.5 | 6 |
| 6709 | Identifying clusters as lowâ€¦lying minimaâ€¦ efficiency of stochastic and genetic algorithms using inexpensive electronic structure levels. <i>Journal of Computational Chemistry</i> , 2012, 33, 502-508. | 1.5 | 14 |
| 6710 | Mechanisms of the cascade synthesis of substituted 4â€¦aminoâ€¦1,2,4â€¦triazolâ€¦one from huisgen zwitterion and aldehyde hydrazone: A DFT study. <i>Journal of Computational Chemistry</i> , 2012, 33, 715-722. | 1.5 | 22 |
| 6711 | Structural and static electric response properties of highly symmetric lithiated silicon cages: Theoretical predictions. <i>Journal of Computational Chemistry</i> , 2012, 33, 1068-1079. | 1.5 | 26 |
| 6712 | On the Accuracy of DFT Methods in Reproducing Ligand Substitution Energies for Transition Metal Complexes in Solution: The Role of Dispersive Interactions. <i>ChemPhysChem</i> , 2012, 13, 562-569. | 1.0 | 58 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6713 | Silver Melonates and Coordination Modes of the Multidentate [C ₆ N ₇ (NCN) ₃] ³⁻ Anion. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 978-986. | 1.0 | 4 |
| 6714 | Anthracene- ^{1,2,3} -Triazole-Linked Bispyridinium Amide for Selective Sensing of H ₂ PO ₄ ⁻ by Fluorescence and Gel Formation. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 1311-1317. | 1.2 | 30 |
| 6715 | Cu-Catalyzed Enantioselective 1,4-Additions of Aryl Grignard Reagents to Cyclohexenone in the Presence of TADDOL-Derived Phosphane-Phosphite Ligands. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 1179-1185. | 1.2 | 23 |
| 6716 | Facial Selectivity in the Diels-Alder Reactions of 2,2-Disubstituted Cyclopent-4-ene-1,3-dione Derivatives and a Computational Examination of the Facial Selectivity of the Diels-Alder Reactions of Structurally Related Dienes and Dienophiles. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 1186-1194. | 1.2 | 7 |
| 6717 | A Cyclobutene-1,2-bis(imidazolium) Salt as Preligand for Palladium-Catalyzed Cross-Coupling Reactions: Properties and Applications. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 754-763. | 1.2 | 5 |
| 6718 | Computational study on the recombination reaction between benzyl and propargyl radicals. <i>International Journal of Chemical Kinetics</i> , 2012, 44, 206-218. | 1.0 | 63 |
| 6719 | Gas-phase doubly charged complexes of cyclic peptides with copper in +1, +2 and +3 formal oxidation states: formation, structures and electron capture dissociation. <i>Journal of Mass Spectrometry</i> , 2012, 47, 208-220. | 0.7 | 17 |
| 6720 | Low Temperature Studies of Iron-Catalyzed Cross-Coupling of Alkyl Grignard Reagents with Aryl Electrophiles. <i>Advanced Synthesis and Catalysis</i> , 2012, 354, 448-456. | 2.1 | 43 |
| 6721 | Integrating computational methods to retrofit enzymes to synthetic pathways. <i>Biotechnology and Bioengineering</i> , 2012, 109, 572-582. | 1.7 | 32 |
| 6722 | Highly Efficient Aerobic Oxidative Hydroxylation of Arylboronic Acids: Photoredox Catalysis Using Visible Light. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 784-788. | 7.2 | 442 |
| 6723 | Linking Ion and Neutral Chemistry in C-H Bond Electrophilic Activation: Generation and Detection of HO ₂ [·] Reactive Radicals in the Gas Phase. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 1455-1458. | 7.2 | 6 |
| 6724 | Is graphene aromatic?. <i>Nano Research</i> , 2012, 5, 117-123. | 5.8 | 106 |
| 6725 | Exact decoupling of the relativistic Fock operator. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1. | 0.5 | 238 |
| 6726 | Low-lying electronic excitations and optical absorption spectra of the black dye sensitizer: a first-principles study. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1. | 0.5 | 9 |
| 6727 | Quantum mechanical calculations of the vibrational spectra of quartz- and rutile-type GeO ₂ . <i>Physics and Chemistry of Minerals</i> , 2012, 39, 47-55. | 0.3 | 32 |
| 6728 | Environment-induced stabilization of hydrogen-bonded dimers in crystal of lysine (5-methyl-1H-[1,2,4]triazol-3-ylsulfanyl)-acetate. <i>Structural Chemistry</i> , 2012, 23, 581-586. | 1.0 | 3 |
| 6729 | Ga ₂ Te ₃ and Ga ₃ Te ₂ clusters: understanding their structures, vibrational and energetic features using DFT and ab initio methods. <i>Journal of Materials Science</i> , 2012, 47, 4332-4341. | 1.7 | 2 |
| 6730 | Ab initio and DFT conformational study on N-nitrosodiethylamine, (C ₂ H ₅) ₂ N-N=O. <i>Journal of Molecular Modeling</i> , 2012, 18, 339-350. | 0.8 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6731 | Computational characterization of the molecular structure and properties of Dye 7 for organic photovoltaics. <i>Journal of Molecular Modeling</i> , 2012, 18, 835-842. | 0.8 | 2 |
| 6732 | Perturbing Peptide Cation-Radical Electronic States by Thioxoamide Groups: Formation, Dissociations, and Energetics of Thioxopeptide Cation-Radicals. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1265-1275. | 1.1 | 7 |
| 6733 | Donor-Substituted Octacyano[4]dendralenes: Investigation of π -Electron Delocalization in Their Radical Ions. <i>Journal of Organic Chemistry</i> , 2013, 78, 1760-1767. | 1.7 | 27 |
| 6734 | Reactivity of amines with hypochlorous acid: Computational study of steric, electronic, and medium effects. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 881-890. | 1.0 | 14 |
| 6735 | DFT, FT-Raman, FTIR, NMR, and UV-Vis studies of a hetarylazo indole dye. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 683-689. | 1.0 | 10 |
| 6736 | Assessing the performance of computational methods for the prediction of the ground state structure of a cyclic decapeptide. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 808-814. | 1.0 | 14 |
| 6737 | Linearity condition for orbital energies in density functional theory (IV): Determination of range-determining parameter. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 245-251. | 1.0 | 6 |
| 6738 | A quantum chemistry study of Ds-Pa unnatural DNA base pair. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 504-509. | 1.0 | 2 |
| 6739 | Inverse sandwich complexes based on low-valent group 13 elements and cyclobutadiene: A theoretical investigation on E_4H_4 ($E = Al, Ga, In, Tl$). <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1018-1025. | 1.0 | 7 |
| 6740 | Computational simulations of hydrolysis of phosphazene oligomer utilizing atom-centered density matrix propagation. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 63-70. | 1.0 | 20 |
| 6741 | Theoretical study of gas phase reactions of important SOA intermediates: (<i>cis</i> and <i>trans</i>) BEPOX and β -EPOX with OH radical. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1162-1170. | 1.0 | 0 |
| 6742 | The choice of the exchange-correlation functional for the determination of the jahn-teller parameters by the density functional theory. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 859-864. | 1.0 | 11 |
| 6743 | Computational study of the covalent bonding of microcystins to cysteine residues a reaction involved in the inhibition of the PPP family of protein phosphatases. <i>FEBS Journal</i> , 2013, 280, 674-680. | 2.2 | 46 |
| 6744 | Experimental and quantum chemical studies of a novel synthetic prenylated chalcone. <i>Chemistry Central Journal</i> , 2013, 7, 17. | 2.6 | 11 |
| 6745 | Conducting properties of new heterometallic one-dimensional coordination polymers derived from 1-nitroethylene-2,2-dithiolate (NED $^{2-}$) ligand and their I 2 -doped products. <i>Synthetic Metals</i> , 2013, 176, 65-69. | 2.1 | 1 |
| 6746 | Interactions between Methane and Polycyclic Aromatic Hydrocarbons: A High Accuracy Benchmark Study. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 370-389. | 2.3 | 36 |
| 6747 | Crystal structure of the polycyclic oxidation product of 1 $^{\beta}$ -phthalazinylhydrazone of 2-formylpyrrole. <i>Journal of Structural Chemistry</i> , 2013, 54, 619-623. | 0.3 | 5 |
| 6748 | Potential energy curves and calculations of spectroscopic constants for the ground state of AlC and AlN. <i>Journal of Structural Chemistry</i> , 2013, 54, 250-254. | 0.3 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6749 | The quest for a better system for evaluating pi-electron substituent constant: a comparison of benzoic, acrylic and triaene, pentaene, heptafulvene-based carboxylic acids. A computational study. Journal of Physical Organic Chemistry, 2013, 26, 892-897. | 0.9 | 3 |
| 6750 | Parameterization of Halogens for the Density-Functional Tight-Binding Description of Halide Hydration. Journal of Chemical Theory and Computation, 2013, 9, 3321-3332. | 2.3 | 12 |
| 6751 | Synthesis, characterization, and biological studies of emissive rhenium-glutamine conjugates. Journal of Biological Inorganic Chemistry, 2013, 18, 831-844. | 1.1 | 18 |
| 6752 | DFT insight into o-semiquinone radicals and Ca ²⁺ ion interaction: structure, g tensor, and stability. Theoretical Chemistry Accounts, 2013, 132, 1. | 0.5 | 13 |
| 6753 | Organometallic copper I, II or III species in an intramolecular dechlorination reaction. Theoretical Chemistry Accounts, 2013, 132, 1. | 0.5 | 1 |
| 6754 | Dispersion-corrected Rung 3.5 density functionals. Theoretical Chemistry Accounts, 2013, 132, 1. | 0.5 | 1 |
| 6755 | A B3LYP study on the C-H activation in propane by neutral and +1 charged low-energy platinum clusters with 2-6 atoms. Reaction Kinetics, Mechanisms and Catalysis, 2013, 109, 315-333. | 0.8 | 9 |
| 6756 | Comparative vibrational spectroscopic studies, HOMO-LUMO and NBO analysis of N-(phenyl)-2,2-dichloroacetamide, N-(2-chloro phenyl)-2,2-dichloroacetamide and N-(4-chloro) Tj ETQq1 1 0.784314 rjBT /Overlock 10 T Chemistry, 2013, 1016, 8-21. | 1.1 | 116 |
| 6757 | Luminescent biscyclometalated arylpyridine iridium(iii) complexes with 4,4-bi-1,2,3-triazolyl ancillary ligands. Dalton Transactions, 2013, 42, 13527. | 1.6 | 41 |
| 6758 | Size dependence of the optical gap of small-silicon quantum dots: Ab initio and empirical correlation schemes. Microelectronic Engineering, 2013, 112, 231-234. | 1.1 | 8 |
| 6759 | Aromatic properties of 8-hydroxyquinoline and its metal complexes. Open Chemistry, 2013, 11, 655-663. | 1.0 | 8 |
| 6760 | A correlated ab initio quantum chemical study of the interaction of the Na ⁺ , Mg ²⁺ , Ca ²⁺ and Zn ²⁺ ions with the tautomers of cytosine in the presence of polar solvent. Physical Chemistry Chemical Physics, 2013, 15, 12930. | 1.3 | 5 |
| 6761 | Theoretical Studies on Intramolecular C-H Amination of Biaryl Azides Catalyzed by Four Different Late Transition Metals. Organometallics, 2013, 32, 415-426. | 1.1 | 37 |
| 6762 | Computational Investigation of Brook-Type Silabenzenes and Their Possible Formation through [1,3]-Si-O Silyl Shifts. Organometallics, 2013, 32, 16-28. | 1.1 | 12 |
| 6763 | Phase Behavior and Molecular Dynamics Simulation Studies of New Aqueous Two-Phase Separation Systems Induced by HEPES Buffer. Journal of Physical Chemistry B, 2013, 117, 563-582. | 1.2 | 28 |
| 6764 | Uniform Treatment of Solute-Solvent Dispersion in the Ground and Excited Electronic States of the Solute Based on a Solvation Model with State-Specific Polarizability. Journal of Chemical Theory and Computation, 2013, 9, 3649-3659. | 2.3 | 59 |
| 6765 | Theoretical Design of pi-Conjugated Heteropolycyclic Compounds Containing a Tricoordinated Boron Center. Journal of Physical Chemistry C, 2013, 117, 14999-15008. | 1.5 | 13 |
| 6766 | Gold-Catalyzed Highly Diastereoselective Synthesis of Functionalized 3,4-Disubstituted Butyrolactams via Phosphatoyloxy or Carbonate Double Migrations. Advanced Synthesis and Catalysis, 2013, 355, 2037-2043. | 2.1 | 22 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6767 | Spectroscopic characterization of cadion: UV-vis, resonance Raman and DFT calculations of a versatile metal complexing agent. <i>Journal of Raman Spectroscopy</i> , 2013, 44, 567-572. | 1.2 | 3 |
| 6768 | Theoretical Study of the Oxidation of Phenolates by the [Cu ₂ O ₂](N ₂) ²⁺ tert-butylethylenediamine ₂ complex. <i>Chemistry - A European Journal</i> , 2013, 19, 1942-1954. | 4.1 | 20 |
| 6769 | Linear-scaling self-consistent field methods for large molecules. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013, 3, 614-636. | 6.2 | 88 |
| 6770 | Molecular Design of UV-vis Absorption and Emission Properties in Organic Fluorophores: Toward Larger Bathochromic Shifts, Enhanced Molar Extinction Coefficients, and Greater Stokes Shifts. <i>Journal of Physical Chemistry C</i> , 2013, 117, 16584-16595. | 1.5 | 209 |
| 6771 | Synthesis, NMR spectroscopic characterization and structure of a divinylsilazane(triphenylphosphine)platinum(0) complex: observation of isotope-induced chemical shifts ¹ P ^{12/13} C(¹⁹⁵ Pt). <i>Magnetic Resonance in Chemistry</i> , 2013, 51, 283-291. | 1.1 | 2 |
| 6772 | Effects of Metal Coordination on the π-System of the 2,5-Bis-((pyrrolidino)-methyl)-pyrrole Pincer Ligand. <i>Inorganic Chemistry</i> , 2013, 52, 9539-9548. | 1.9 | 23 |
| 6773 | Ligand field density functional theory calculation of the 4f ₂ → 4f ₁₅ d ₁ transitions in the quantum cutter Cs ₂ KYF ₆ :Pr ³⁺ . <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13902. | 1.3 | 50 |
| 6774 | Utilization of nicotinonitrile-2-thiol in the synthesis of new thiepino[2,3-b]pyridine derivative as an in vitro novel antitumor potent. <i>Medicinal Chemistry Research</i> , 2013, 22, 1674-1678. | 1.1 | 2 |
| 6775 | Malonic Acid Half Oxyesters and Thioesters: Solvent-Free Synthesis and DFT Analysis of Their Enols. <i>Organic Letters</i> , 2013, 15, 3805-3807. | 2.4 | 7 |
| 6776 | Crystal structure of bis-Isonicotinoyl hydrazone of 2,5-diformylpyrrole. <i>Journal of Structural Chemistry</i> , 2013, 54, 592-597. | 0.3 | 3 |
| 6777 | Nuclear wastefrom materials: Atomistic simulation case studies. <i>Journal of Nuclear Materials</i> , 2013, 441, 29-39. | 1.3 | 45 |
| 6778 | Predicting Intrinsic Clearance for Drugs and Drug Candidates Metabolized by Aldehyde Oxidase. <i>Molecular Pharmaceutics</i> , 2013, 10, 1262-1268. | 2.3 | 41 |
| 6779 | Efficient and stable DSSC sensitizers based on substituted dihydroindolo[2,3-b]carbazole donors with high molar extinction coefficients. <i>Journal of Materials Chemistry A</i> , 2013, 1, 11295. | 5.2 | 87 |
| 6780 | A DFT study of the vicinal ³ J(119Sn,13C) and ³ J(119Sn,1H) coupling constants in trimethyl- and chlorodimethylstannyl propanoates. <i>Journal of Organometallic Chemistry</i> , 2013, 724, 139-146. | 0.8 | 8 |
| 6781 | Thermodynamic and aromaticity studies for the assessment of the halogen-cyano interactions on iodobenzonitrile. <i>Journal of Chemical Thermodynamics</i> , 2013, 65, 204-212. | 1.0 | 5 |
| 6782 | Reaction of Dimethyl Ether with Hydroxyl Radicals: Kinetic Isotope Effect and Prereactive Complex Formation. <i>Journal of Physical Chemistry A</i> , 2013, 117, 8343-8351. | 1.1 | 47 |
| 6783 | First Principle Approach to Solvation by Methylimidazolium-Based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2013, 117, 553-562. | 1.2 | 21 |
| 6784 | Computational Prediction for Singlet- and Triplet-Transition Energies of Charge-Transfer Compounds. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3872-3877. | 2.3 | 312 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6785 | Dancing multiplicity states supported by a carboxylated group in dicopper structures bonded to O ₂ . <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1. | 0.5 | 12 |
| 6786 | Investigating the Ritter Type Reaction of β -Methylene α -Hydroxy Esters in Acidic Medium: Evidence for the Intermediacy of an Allylic Cation. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 5180-5187. | 1.2 | 5 |
| 6787 | Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in <i>para</i> -nitroaniline. <i>Molecular Physics</i> , 2013, 111, 1235-1248. | 0.8 | 79 |
| 6788 | Relating normal vibrational modes to local vibrational modes: benzene and naphthalene. <i>Journal of Molecular Modeling</i> , 2013, 19, 2865-2877. | 0.8 | 35 |
| 6789 | Tests of Exchange-Correlation Functional Approximations Against Reliable Experimental Data for Average Bond Energies of 3d Transition Metal Compounds. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3965-3977. | 2.3 | 95 |
| 6790 | Structure-Reactivity Relationships in the Hydrogenation of Carbon Dioxide with Ruthenium Complexes Bearing Pyridinylazoloto Ligands. <i>Chemistry - A European Journal</i> , 2013, 19, 7825-7834. | 1.7 | 33 |
| 6791 | Selective activation of C-F and C-H bonds with iron complexes, the relevant mechanism study by DFT calculations and study on the chemical properties of hydrido iron complex. <i>Dalton Transactions</i> , 2013, 42, 3417-3428. | 1.6 | 16 |
| 6792 | Effects of London dispersion correction in density functional theory on the structures of organic molecules in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16031. | 1.3 | 238 |
| 6793 | Theoretical Spectroscopy of the Ni ^{II} Intermediate States in the Catalytic Cycle and the Activation of [NiFe] Hydrogenases. <i>ChemBioChem</i> , 2013, 14, 1898-1905. | 1.3 | 56 |
| 6794 | Methane hydrates and their HF doped analogues. <i>Chemical Physics Letters</i> , 2013, 578, 110-114. | 1.2 | 8 |
| 6795 | Direct measurement and modulation of single-molecule coordinative bonding forces in a transition metal complex. <i>Nature Communications</i> , 2013, 4, 2121. | 5.8 | 43 |
| 6796 | Chiroptical Properties of Carbo[6]Helicene Derivatives Bearing Extended π -Conjugated Cyano Substituents. <i>Chirality</i> , 2013, 25, 455-465. | 1.3 | 36 |
| 6797 | Can self-assembly of copper(ii) picolinamide building blocks be controlled?. <i>CrystEngComm</i> , 2013, 15, 8074. | 1.3 | 9 |
| 6798 | Dimetallaboranes with Polyhedral Surface Metal-Metal Multiple Bonds: Deltahedral Dirhenaboranes with Pentalenedirhenium Vertices. <i>Organometallics</i> , 2013, 32, 4002-4008. | 1.1 | 8 |
| 6799 | Relativistic density functional theory modeling of plutonium and americium higher oxide molecules. <i>Journal of Chemical Physics</i> , 2013, 139, 034307. | 1.2 | 19 |
| 6800 | Mechanistic aspects of the reaction of dimedone derivatives with sulfenic acids and other sulfur compounds—a computational study. <i>Tetrahedron</i> , 2013, 69, 7243-7252. | 1.0 | 7 |
| 6801 | Nucleophilic Halogenations of Diazo Compounds, a Complementary Principle for the Synthesis of Halodiazo Compounds: Experimental and Theoretical Studies. <i>Journal of Organic Chemistry</i> , 2013, 78, 7488-7497. | 1.7 | 42 |
| 6802 | A new family of hybrid density functionals. <i>Chemical Physics Letters</i> , 2013, 580, 166-171. | 1.2 | 104 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 6803 | Controlling dye aggregation, injection energetics and catalytic recombination in organic sensitizer based dye cells using a single electrolyte additive. <i>Energy and Environmental Science</i> , 2013, 6, 3046. | 15.6 | 15 |
| 6804 | Enantiomeric separation of d- and l-lactic acid enantiomers by use of nanotubular cyclicpeptides: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2013, 1020, 163-169. | 1.1 | 7 |
| 6805 | Giant Faraday Rotation in Mesogenic Organic Molecules. <i>Chemistry of Materials</i> , 2013, 25, 1139-1143. | 3.2 | 44 |
| 6806 | Influence of fluorination on UV spectra of polyurethane structural fragments. <i>Journal of Applied Spectroscopy</i> , 2013, 80, 319-325. | 0.3 | 0 |
| 6807 | 2-(9,10-Anthraquinon-2-yl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazole-3-oxide-1-oxyl: polymorphism in a conjugated anthraquinone-substituted nitronyl nitroxide. <i>Chemical Communications</i> , 2013, 49, 3345. | 2.2 | 4 |
| 6808 | QM/MM study of the conversion mechanism of lysine to methylornithine catalyzed by methylornithine synthase (PylB). <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1. | 0.5 | 9 |
| 6809 | Chemo- and diastereoselective tandem dual oxidation of B(pin)-substituted allylic alcohols: synthesis of B(pin)-substituted epoxy alcohols, 2-keto-anti-1,3-diols and dihydroxy-tetrahydrofuran-3-ones. <i>Chemical Science</i> , 2013, 4, 3946. | 3.7 | 11 |
| 6810 | A dispersion-corrected density functional theory study of hexamers of formic acid. <i>Canadian Journal of Chemistry</i> , 2013, 91, 527-528. | 0.6 | 3 |
| 6811 | The mechanism for the hydrogenation of ketones catalyzed by KnÃ¶lker's iron-catalyst. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 5264. | 1.5 | 46 |
| 6812 | Aromatic interactions in asymmetric catalysis: control of enantioselectivity in Diels-Alder reactions catalysed by camphor-derived hydrazides. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 5226. | 1.5 | 10 |
| 6813 | Comparison of TD-DFT Methods for the Calculation of Two-Photon Absorption Spectra of Oligophenylvinylenes. <i>Journal of Physical Chemistry C</i> , 2013, 117, 18170-18189. | 1.5 | 68 |
| 6814 | Computational Analysis of ^{47/49} Ti NMR Shifts and Electric Field Gradient Tensors of Half-Titanocene Complexes: Structure-Bonding-Property Relationships. <i>Chemistry - A European Journal</i> , 2013, 19, 12018-12033. | 1.7 | 12 |
| 6815 | Theoretical investigations of the structures and electronic spectra of 8-hydroxylquinoline derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 115, 464-468. | 2.0 | 0 |
| 6816 | The role of Hartree-Fock exchange in the simulation of X-ray absorption spectra: A study of photoexcited. <i>Chemical Physics Letters</i> , 2013, 580, 179-184. | 1.2 | 43 |
| 6817 | Agarsenone, a Cadinane Sesquiterpenoid from <i>Commiphora erythraea</i> . <i>Journal of Natural Products</i> , 2013, 76, 1254-1259. | 1.5 | 21 |
| 6818 | Experimental and computational study of the complexation of Adamantyl glycosides with β -cyclodextrin. <i>Tetrahedron</i> , 2013, 69, 8051-8063. | 1.0 | 12 |
| 6819 | Recent Progress in Density Functional Methodology for Biomolecular Modeling. <i>Structure and Bonding</i> , 2013, , 1-64. | 1.0 | 9 |
| 6820 | Polymorphic Co-crystals from Polymorphic Co-crystal Formers: Competition between Carboxylic Acid-Pyridine and Phenol-Pyridine Hydrogen Bonds. <i>Crystal Growth and Design</i> , 2013, 13, 3935-3952. | 1.4 | 80 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6821 | DFT study of electronic band structure of alternating triphenylamine-fluorene copolymers. <i>Polymer</i> , 2013, 54, 2535-2543. | 1.8 | 12 |
| 6822 | Mechanistic Study of the Rhodium-Catalyzed [3+2+2] Carbocyclization of Alkenylidenecyclopropanes with Alkynes. <i>Chemistry - an Asian Journal</i> , 2013, 8, 2262-2273. | 1.7 | 28 |
| 6823 | Thermodynamic, kinetic and electronic structure aspects of a charge-transfer active bichromophoric organofullerene. <i>Journal of Chemical Sciences</i> , 2013, 125, 237-246. | 0.7 | 1 |
| 6824 | Synthesis and theoretic calculations of benzoxazoles and docking studies of their interactions with triosephosphate isomerase. <i>Medicinal Chemistry Research</i> , 2013, 22, 2768-2777. | 1.1 | 4 |
| 6825 | Synthesis and mesomorphic behaviour of achiral four-ring unsymmetrical bent-core liquid crystals: Nematic phases. <i>Journal of Molecular Structure</i> , 2013, 1049, 78-89. | 1.8 | 20 |
| 6826 | Production of ions at high energy and its role in extraterrestrial environments. <i>Rendiconti Lincei</i> , 2013, 24, 53-65. | 1.0 | 45 |
| 6827 | Comparative assessment of density functionals for excited-state dipole moments. <i>Chemical Physics Letters</i> , 2013, 584, 58-62. | 1.2 | 9 |
| 6828 | Accelerating influence of the gem-difluoromethylene group in a ring-closing olefin metathesis reaction. A Thorpe-Ingold effect?. <i>Chemical Communications</i> , 2013, 49, 7201. | 2.2 | 21 |
| 6829 | Spectroscopic (FT-IR, FT-Raman, UV and NMR) investigation, conformational stability, NLO properties, HOMO-LUMO and NBO analysis of hydroxyquinoline derivatives by density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 114, 449-474. | 2.0 | 32 |
| 6830 | Rational Design of Strongly Blue-Emitting Cuprous Complexes with Thermally Activated Delayed Fluorescence and Application in Solution-Processed OLEDs. <i>Chemistry of Materials</i> , 2013, 25, 3910-3920. | 3.2 | 241 |
| 6831 | A Guided Self-Consistent-Field Method for Excited-State Wave Function Optimization: Applications to Ligand-Field Transitions in Transition-Metal Complexes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3933-3938. | 2.3 | 24 |
| 6832 | A Theoretical Study of Formation Routes and Dimerization of Methanimine and Implications for the Aerosols Formation in the Upper Atmosphere of Titan. <i>Lecture Notes in Computer Science</i> , 2013, , 47-56. | 1.0 | 16 |
| 6833 | Spontaneous formation of branched nanochains from room temperature molten amides: visible and near-IR active, SERS substrates for non-fluorescent and fluorescent analytes. <i>RSC Advances</i> , 2013, 3, 8356. | 1.7 | 14 |
| 6834 | FT-IR, FT-Raman, NMR spectra and DFT simulations of 4-(4-fluoro-phenyl)-1H-imidazole. <i>Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)</i> , 2013, 114, 525-536. | 0.2 | 24 |
| 6835 | Reactivity of Dicoordinated Stannylones (Sn 0) versus Stannylones (Sn II): An Investigation Using DFT-Based Reactivity Indices. <i>ChemPhysChem</i> , 2013, 14, 3233-3247. | 1.0 | 6 |
| 6836 | Water Cluster Confinement and Methane Adsorption in the Hydrophobic Cavities of a Fluorinated Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2013, 135, 12615-12626. | 6.6 | 114 |
| 6837 | Site Preferences of Carboxyl Groups on the Periphery of Graphene and Their Characteristic IR Spectra. <i>Journal of Physical Chemistry C</i> , 2013, 117, 18206-18215. | 1.5 | 12 |
| 6838 | Marine natural products from the deep Pacific as potential non-linear optical chromophores. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14814. | 1.3 | 9 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6839 | Stereoselective synthesis of highly functionalized tetrahydrocarbazoles through a domino Michaelâ€“Henry reaction: an easy access to four contiguous chiral centers. <i>RSC Advances</i> , 2013, 3, 10644. | 1.7 | 26 |
| 6840 | Geometrical Correction for the Inter- and Intramolecular Basis Set Superposition Error in Periodic Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 9282-9292. | 1.1 | 123 |
| 6841 | Theoretical studies of iron(iii)-catalyzed intramolecular Câ€“H amination of azides. <i>Dalton Transactions</i> , 2013, 42, 14369. | 1.6 | 17 |
| 6842 | DFT-Based Quantum Chemical Studies on Conformational, Electronic and Antioxidant Properties of Isobavachalcone and 4-Hydroxyderricin. <i>Food Biophysics</i> , 2013, 8, 250-255. | 1.4 | 12 |
| 6843 | The study of performance of DFT functional for van der Waals interactions. <i>Computational and Theoretical Chemistry</i> , 2013, 1004, 56-60. | 1.1 | 3 |
| 6844 | Density functional study of mono-branched and di-branched di-anchoring triphenylamine cyanoacrylic dyes for dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2013, 253, 62-71. | 2.0 | 17 |
| 6845 | How Well Can DFT Reproduce Key Interactions in Zieglerâ€“Natta Systems?. <i>Macromolecular Chemistry and Physics</i> , 2013, 214, 1980-1989. | 1.1 | 40 |
| 6846 | Bond fukui indices: Comparison of frozen molecular orbital and finite differences through mulliken populations. <i>Journal of Computational Chemistry</i> , 2013, 34, 2421-2429. | 1.5 | 14 |
| 6847 | Computational reexamination of the eclipsed conformation in cis-2-tert-butyl-5-(tert-butylsulfonyl)-1,3-dioxane. <i>Structural Chemistry</i> , 2013, 24, 1855-1862. | 1.0 | 8 |
| 6848 | Stability and aromaticity of tautomers and kinetics of proton transfer in 6-methylpentafulvene and its exo-substituted derivatives: a computational study. <i>Structural Chemistry</i> , 2013, 24, 981-991. | 1.0 | 7 |
| 6849 | Theoretical studies on tautomerism of imidazole-2-selenone. <i>Structural Chemistry</i> , 2013, 24, 1215-1227. | 1.0 | 11 |
| 6850 | A DFT study of cage compounds: 3, 5, 8, 10, 11, 12-hexanitro-3, 5, 8, 10, 11, 12-hexaazatetracyclo [5.5.1.12,6.04,9] dodecane and its derivatives as high energetic materials. <i>Structural Chemistry</i> , 2013, 24, 1339-1346. | 1.0 | 15 |
| 6851 | A computational investigation of the effect of the double bond on the conformations of seven membered rings. <i>Structural Chemistry</i> , 2013, 24, 243-250. | 1.0 | 3 |
| 6852 | How Theoretical Simulations Can Address the Structure and Activity of Nanoparticles. <i>Topics in Catalysis</i> , 2013, 56, 1262-1272. | 1.3 | 16 |
| 6853 | A DFT Study of Ethylene Hydrogenation Reaction Mechanisms on Ni ₁₃ Nanocluster. <i>Topics in Catalysis</i> , 2013, 56, 789-793. | 1.3 | 3 |
| 6854 | On the Way to Biofuels from Furan: Discriminating Dielsâ€“Alder and Ring-Opening Mechanisms. <i>ACS Catalysis</i> , 2013, 3, 2012-2019. | 5.5 | 39 |
| 6855 | Ab Initio Prediction of Proton NMR Chemical Shifts in Imidazolium Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3186-3197. | 1.2 | 56 |
| 6856 | TD-DFT studies on electronic and spectral properties of platinum(II) complexes with phenol and pyridine groups. <i>Chemical Research in Chinese Universities</i> , 2013, 29, 361-365. | 1.3 | 6 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6857 | Understanding and Reducing Errors in Density Functional Calculations. <i>Physical Review Letters</i> , 2013, 111, 073003. | 2.9 | 271 |
| 6858 | Predicting the Stability Constants of Metal-Ion Complexes from First Principles. <i>Inorganic Chemistry</i> , 2013, 52, 10347-10355. | 1.9 | 57 |
| 6859 | Unraveling the Origin of the Relative Stabilities of Group 14 M_{2N}^{2+} ($M, N = C, Si, Ge, Sn, \text{ and } Pb$) Isomer Clusters. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10462-10469. | 1.1 | 13 |
| 6860 | Is the Tamm-Dancoff Approximation Reliable for the Calculation of Absorption and Fluorescence Band Shapes?. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4517-4525. | 2.3 | 95 |
| 6861 | Structure of Au_{40}^{+1} in the gas phase: A joint geometry relaxed ab initio calculations and vibrationally resolved photoelectron imaging investigation. <i>Journal of Chemical Physics</i> , 2013, 139, 094306. | 1.2 | 10 |
| 6862 | Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Applications and Insights. , 2013, , 1-57. | | 1 |
| 6863 | Structure and Vibrational Spectra. , 2013, , 971-987. | | 1 |
| 6864 | Computational Methods for Solids. , 2013, , 59-87. | | 2 |
| 6865 | Linear and Nonlinear Optical Properties of Expanded Porphyrins: A DMRG Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7804-7809. | 1.1 | 21 |
| 6866 | Thorough theoretical search of conformations of neutral, protonated and deprotonated glutamine in gas phase. <i>Computational and Theoretical Chemistry</i> , 2013, 1020, 14-21. | 1.1 | 11 |
| 6867 | Rigid triarylamine-based "A structural organic sensitizers for solar cells: the significant enhancement of open-circuit photovoltage with a long alkyl group. <i>RSC Advances</i> , 2013, 3, 22544. | 1.7 | 19 |
| 6868 | Cyclometalated platinum(ii) with ethynyl-linked azobenzene ligands: an original switching mode. <i>Dalton Transactions</i> , 2013, 42, 16773. | 1.6 | 14 |
| 6869 | The influence of substitution in the quinoxaline nucleus on 1,3-dipolar cycloaddition reactions: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2013, 1013, 116-122. | 1.1 | 8 |
| 6870 | DFT calculation of the electronic properties of fluorene-1,3,4-thiadiazole oligomers. <i>Journal of Molecular Modeling</i> , 2013, 19, 3537-3542. | 0.8 | 9 |
| 6871 | Comparative studies for evaluation of CO ₂ fixation in the cavity of the Rubisco enzyme using QM, QM/MM and linear-scaling DFT methods. <i>Journal of Molecular Modeling</i> , 2013, 19, 2329-2334. | 0.8 | 12 |
| 6872 | Role of gold in a complex cascade reaction involving two electrocyclization steps. <i>Journal of Molecular Modeling</i> , 2013, 19, 1981-1984. | 0.8 | 1 |
| 6873 | Assessing the quantum mechanical level of theory for prediction of linear and nonlinear optical properties of push-pull organic molecules. <i>Journal of Molecular Modeling</i> , 2013, 19, 2079-2090. | 0.8 | 18 |
| 6874 | Structural characterization of the (MeSH) ₄ potential energy surface. <i>Journal of Molecular Modeling</i> , 2013, 19, 2173-2181. | 0.8 | 13 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6875 | Computational Modeling of Isoindigo-Based Polymers Used in Organic Solar Cells. <i>Journal of Physical Chemistry C</i> , 2013, 117, 17940-17954. | 1.5 | 27 |
| 6876 | On the sensitivity of hard X-ray spectroscopies to the chemical state of Br. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 11088. | 1.3 | 13 |
| 6877 | Development and application of effective pairwise potentials for UO_2^{n+} , NpO_2^{n+} , PuO_2^{n+} , and AmO_2^{n+} ($n = 1, 2$) ions with water. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 15954. | 1.3 | 42 |
| 6878 | Theoretical Study on Ruthenium-Catalyzed Hydrocarboxylative Dimerization of Phenylacetylene with Acetic Acid Leading to (1 <i>i></i> E</i>,3<i>E</i>)-1,4-Diphenyl-1,3-butadienyl Acetate. <i>Organometallics</i> , 2013, 32, 5201-5211. | 1.1 | 8 |
| 6879 | Negative ion fragmentations of disulfideâ€containing crossâ€linking reagents are competitive with aspartic acid sideâ€chainâ€induced cleavages. <i>Rapid Communications in Mass Spectrometry</i> , 2013, 27, 238-248. | 0.7 | 6 |
| 6880 | Configurational, LFDFT and NBO analysis of chromium(III) complexes of edta-type ligands. <i>Polyhedron</i> , 2013, 55, 131-143. | 1.0 | 15 |
| 6881 | Critical Test of Some Computational Chemistry Methods for Prediction of Gas-Phase Acidities and Basicities. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3947-3958. | 2.3 | 38 |
| 6882 | Ï€ Donation and Its Effects on the Excited-State Lifetimes of Luminescent Platinum(II) Terpyridine Complexes in Solution. <i>Inorganic Chemistry</i> , 2013, 52, 8476-8482. | 1.9 | 14 |
| 6883 | Synthesis and Isomerization of N-Fused Tetraphenylporphyrin Ruthenium(II) Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 9613-9619. | 1.9 | 14 |
| 6884 | Molecular Origins of Dye Aggregation and Complex Formation Effects in Coumarin 343. <i>Journal of Physical Chemistry C</i> , 2013, 117, 14723-14730. | 1.5 | 43 |
| 6885 | On the calculation of the vibrational frequencies of C_6H_4 . <i>Chemical Physics Letters</i> , 2013, 566, 1-3. | 1.2 | 5 |
| 6886 | Calculation of the $4f1\hat{t}^*4f05d1$ transitions in Ce^{3+} -doped systems by Ligand Field Density Functional Theory. <i>Chemical Physics Letters</i> , 2013, 588, 260-266. | 1.2 | 36 |
| 6887 | Through-space and through-bridge interactions in the correlation analysis of chemical bonds. <i>Computational and Theoretical Chemistry</i> , 2013, 1026, 72-77. | 1.1 | 8 |
| 6888 | Molecular structure, vibrational and EPR spectra of Cu(II) chloride complex of 4-amino-1-methylbenzene combined with quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2013, 1054-1055, 76-82. | 1.8 | 7 |
| 6889 | Tuning Anionâ€Functionalized Ionic Liquids for Improved SO_2 Capture. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 10620-10624. | 7.2 | 152 |
| 6890 | ABSORPTION SPECTRA OF NUCLEIC ACID BASES IN WATER ENVIRONMENT: INSIGHTS INTO FROM COMBINED QM/MM AND CLUSTER-CONTINUUM MODEL CALCULATIONS. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1341013. | 1.8 | 14 |
| 6891 | Mechanism of the Methyltrioxorheniumâ€Catalyzed Deoxydehydration of Polyols: A New Pathway Revealed. <i>Chemistry - A European Journal</i> , 2013, 19, 3827-3832. | 1.7 | 71 |
| 6892 | Mechanism of Copper(I)â€Catalyzed Allylic Alkylation of Phosphorothioate Esters: Influence of the Leaving Group on ï± Regioselectivity. <i>Chemistry - A European Journal</i> , 2013, 19, 14126-14142. | 1.7 | 14 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6893 | The Two Faces of Hydrogen-Bond Strength on Triple AAA-DDD Arrays. <i>ChemPhysChem</i> , 2013, 14, 3994-4001. | 1.0 | 14 |
| 6894 | Gas-phase structures of phosphopeptide ions: A difficult case. <i>International Journal of Mass Spectrometry</i> , 2013, 354-355, 249-256. | 0.7 | 24 |
| 6895 | Energy and entropy at play in competitive dissociations: The case of uneven positional dissociation of ionized triacylglycerides. <i>International Journal of Mass Spectrometry</i> , 2013, 352, 77-86. | 0.7 | 16 |
| 6896 | Selective and Practical Oxidation of Sulfides to Diastereopure Sulfoxides: A Combined Experimental and Computational Investigation. <i>Advanced Synthesis and Catalysis</i> , 2013, 355, 191-202. | 2.1 | 17 |
| 6897 | C ⁺ -cyclometalated platinum(II) complexes with trifluoromethyl-acetylacetonate ligands – Synthesis and electronic effects. <i>Journal of Organometallic Chemistry</i> , 2013, 730, 37-43. | 0.8 | 16 |
| 6898 | Experimental and theoretical study of the vibrational spectra of 12-thiacrown-4 and 18-thiacrown-6, evaluation of the performance of the different anharmonic force fields compared to the scaled quantum mechanical force fields. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 116, 584-593. | 2.0 | 3 |
| 6899 | Using optimally tuned range separated hybrid functionals in ground-state calculations: Consequences and caveats. <i>Journal of Chemical Physics</i> , 2013, 138, 204115. | 1.2 | 166 |
| 6900 | Mapping of Functional Groups in Metal-Organic Frameworks. <i>Science</i> , 2013, 341, 882-885. | 6.0 | 411 |
| 6901 | A constrained reduced-dimensionality search algorithm to follow chemical reactions on potential energy surfaces. <i>Journal of Chemical Physics</i> , 2013, 138, 214102. | 1.2 | 9 |
| 6902 | Phenylazindole dyes – Part I: The syntheses, characterizations, crystal structures, quantum chemical calculations and antimicrobial properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 113, 314-324. | 2.0 | 13 |
| 6903 | Theoretical studies on the photoisomerization-switchable second-order nonlinear optical responses of DTE-linked polyoxometalate derivatives. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 40, 110-115. | 1.3 | 15 |
| 6904 | On the role of noncovalent interactions in electrocatalysis. Two cases of mediated reductive dehalogenation. <i>Electrochimica Acta</i> , 2013, 110, 619-627. | 2.6 | 9 |
| 6905 | A combined experimental and theoretical study of surface film formation: Effect of oxygen on the reduction mechanism of propylene carbonate. <i>Journal of Power Sources</i> , 2013, 244, 318-327. | 4.0 | 21 |
| 6906 | Electronic states of porphycene-O ₂ complex and photoinduced singlet O ₂ production. <i>Journal of Chemical Physics</i> , 2013, 139, 074307. | 1.2 | 7 |
| 6907 | Computational screening of functionalized zinc porphyrins for dye sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 19478. | 1.3 | 36 |
| 6908 | Synthesis and luminescence properties of biphenyl-type firefly luciferin analogs with a new, near-infrared light-emitting bioluminophore. <i>Tetrahedron</i> , 2013, 69, 9726-9734. | 1.0 | 39 |
| 6909 | 2-Arylideneferroceno[e]cyclohexanones and related 3-aryl-3,3a,4,5-tetrahydroferroceno[g]indazoles: Synthesis, NMR-, DFT- and X-ray analysis. <i>Journal of Organometallic Chemistry</i> , 2013, 726, 79-87. | 0.8 | 4 |
| 6910 | π-Conjugated Molecules Containing Naphtho[2,3-b]thiophene and Their Derivatives: Theoretical Design for Organic Semiconductors. <i>Journal of Physical Chemistry C</i> , 2013, 117, 10175-10184. | 1.5 | 50 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6911 | Luminescent diiridium(III) complex with a bridging biuretato ligand in unprecedented N,N- π^2 :O, π^2 coordination. <i>Journal of Organometallic Chemistry</i> , 2013, 745-746, 341-346. | 0.8 | 6 |
| 6912 | Exploring the correlation between molecular conformation and UV-visible absorption spectra of two-dimensional thiophene-based conjugated polymers. <i>Polymer</i> , 2013, 54, 6489-6499. | 1.8 | 15 |
| 6913 | Molecular Origins of Optoelectronic Properties in Coumarins 343, 314T, 445, and 522B. <i>Journal of Physical Chemistry C</i> , 2013, 117, 14130-14141. | 1.5 | 36 |
| 6914 | A Theoretical DFT-Based and Experimental Study of the Transmetalation Step in Au/Pd-Mediated Cross-Coupling Reactions. <i>Chemistry - A European Journal</i> , 2013, 19, 15290-15303. | 1.7 | 49 |
| 6915 | Quantum chemical analysis of salen-aluminum complexes for organic light emitting diodes. <i>Chemical Physics Letters</i> , 2013, 585, 143-148. | 1.2 | 6 |
| 6916 | Fundamental Reaction Pathway and Free Energy Profile for Butyrylcholinesterase-Catalyzed Hydrolysis of Heroin. <i>Biochemistry</i> , 2013, 52, 6467-6479. | 1.2 | 35 |
| 6917 | A systematic theoretical study of the electronic structures of porphyrin dimers: DFT and TD-DFT calculations on diporphyrins linked by ethane, ethene, ethyne, imine, and azo bridges. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18951. | 1.3 | 38 |
| 6918 | Interaction between Histidine and Zn(II) Metal Ions over a Wide pH as Revealed by Solid-State NMR Spectroscopy and DFT Calculations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 8954-8965. | 1.2 | 48 |
| 6919 | Oxazoline-Based Organocatalyst for Enantioselective Strecker Reactions: A Protocol for the Synthesis of Levamisole. <i>Chemistry - A European Journal</i> , 2013, 19, 14224-14232. | 1.7 | 19 |
| 6920 | A Density Functional Theory Investigation into the Binding of the Antioxidants Ergothioneine and Othiol to Copper. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4057-4065. | 1.1 | 23 |
| 6921 | Systematic Investigation of Organic Photovoltaic Cell Charge Injection/Performance Modulation by Dipolar Organosilane Interfacial Layers. <i>ACS Applied Materials & Interfaces</i> , 2013, 5, 9224-9240. | 4.0 | 29 |
| 6922 | Amine Superbases Stabilized by Extended Hydrogen Bond Networks. <i>Journal of Organic Chemistry</i> , 2013, 78, 10909-10916. | 1.7 | 30 |
| 6923 | A dispersion-corrected density functional theory case study on ethyl acetate conformers, dimer, and molecular crystal. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1. | 0.5 | 18 |
| 6924 | Low temperature X-ray molecular structure, tautomerism and spectral properties of 2,3-dihydroquinoxaline. <i>Journal of Molecular Structure</i> , 2013, 1053, 48-60. | 1.8 | 3 |
| 6925 | Sneaking up on the Criegee intermediate from below: Predicted photoelectron spectrum of the CH ₂ OO ⁻ anion and W3-F12 electron affinity of CH ₂ OO. <i>Chemical Physics Letters</i> , 2013, 585, 15-20. | 1.2 | 13 |
| 6926 | Optical absorption in donor-acceptor polymers - alternating vs. random. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 20016. | 1.3 | 14 |
| 6927 | Isolated catalyst sites on amorphous supports: A systematic algorithm for understanding heterogeneities in structure and reactivity. <i>Journal of Chemical Physics</i> , 2013, 138, 204105. | 1.2 | 41 |
| 6928 | Tin (IV) alkoxide initiator design for poly (d-lactide) synthesis using DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2013, 1020, 121-126. | 1.1 | 15 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6929 | Theoretical investigations of BBS (singlet)→BSB (triplet) transformation on a potential energy surface obtained from neural network fitting. <i>Chemical Physics</i> , 2013, 426, 31-37. | 0.9 | 4 |
| 6930 | On Predicting Mössbauer Parameters of Iron-Containing Molecules with Density-Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5004-5020. | 2.3 | 75 |
| 6931 | A first-principles study on the structural, elastic, electronic, optical, lattice dynamical, and thermodynamic properties of zinc-blende CdX (X= S, Se, and Te). <i>Journal of Alloys and Compounds</i> , 2013, 579, 583-593. | 2.8 | 46 |
| 6932 | Studies on tautomeric stability and equilibrium of 5(4)-substituted-1,2,3 triazoles. I. Electronegativity and resonance effects of substituent. <i>Computational and Theoretical Chemistry</i> , 2013, 1026, 31-37. | 1.1 | 4 |
| 6933 | A DFT study of the Al ₂ Cl ₆ -catalyzed Friedel-Crafts acylation of phenyl aromatic compounds. <i>Journal of Molecular Modeling</i> , 2013, 19, 4947-4958. | 0.8 | 14 |
| 6934 | Reductive Coupling of Azides Mediated by an Iron(II) Bis(alkoxide) Complex. <i>Inorganic Chemistry</i> , 2013, 52, 12335-12337. | 1.9 | 36 |
| 6935 | Synthesis and stereochemistry of new 1,3-thiazolidine systems based on 2-amino-2-(mercaptomethyl)propane-1,3-diol: 4,4-bis(hydroxymethyl)-1,3-thiazolidines and c-5-hydroxymethyl-3-oxa-7-thia-r-1-azabicyclo[3.3.0]octanes. <i>Tetrahedron</i> , 2013, 69, 9966-9985. | 1.0 | 3 |
| 6936 | Two-dimensional stimulated resonance Raman spectroscopy study of the Trp-cage peptide folding. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 19457. | 1.3 | 17 |
| 6937 | Catalytic Mechanism of the Glycyl Radical Enzyme 4-Hydroxyphenylacetate Decarboxylase from Continuum Electrostatic and QC/MM Calculations. <i>Journal of the American Chemical Society</i> , 2013, 135, 14574-14585. | 6.6 | 31 |
| 6938 | Calcium- ²⁺ -Gulonate Complexes: Ca ²⁺ Binding Modes from DFT-MD Simulations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 12105-12112. | 1.2 | 29 |
| 6939 | Achiral unsymmetrical four-ring bent-core liquid crystals with a polar fluoro or chloro end substituent: synthesis and characterisation. <i>Liquid Crystals</i> , 2013, 40, 1105-1115. | 0.9 | 25 |
| 6940 | Interconversion of Metallanaphthalynes and Indenylidene Complexes: A DFT Prediction. <i>Organometallics</i> , 2013, 32, 6271-6276. | 1.1 | 33 |
| 6941 | Physicochemical vs. Vibrational Descriptors for Prediction of Odor Receptor Responses. <i>Molecular Informatics</i> , 2013, 32, 855-865. | 1.4 | 19 |
| 6942 | Controlling the Structure of Reactive Intermediates via Incipient Covalent Bonding with the Counterions: Coexistence of Two Distinct Forms of the C ₆ F ₆ Cation Radical in a Single Crystal. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23568-23574. | 1.5 | 2 |
| 6943 | Assessing the Proton Affinities of N,N- ²⁻ Diamidocarbenes. <i>Journal of Organic Chemistry</i> , 2013, 78, 10452-10458. | 1.7 | 21 |
| 6944 | Mechanism of Iron Carbonyl-Catalyzed Hydrogenation of Ethylene. 1. Theoretical Exploration of Molecular Pathways. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10912-10932. | 1.1 | 13 |
| 6945 | Heteroleptic, Dinuclear Copper(I) Complexes for Application in Organic Light-Emitting Diodes. <i>Chemistry of Materials</i> , 2013, 25, 4471-4486. | 3.2 | 220 |
| 6946 | Copper(I) Complexes Based on Five-Membered P ^{>} N Heterocycles: Structural Diversity Linked to Exciting Luminescence Properties. <i>Inorganic Chemistry</i> , 2013, 52, 13509-13520. | 1.9 | 101 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6947 | Investigation of Magnetic Exchange Pathways in Heterotrinnuclear Manganese(III) Schiff Base Complexes Involving Tetrathiocyanidoplatinate(II) Bridges. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 5781-5789. | 1.0 | 8 |
| 6948 | Reactions of Neutral Platinum Clusters with N_2O and CO. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12175-12183. | 1.1 | 30 |
| 6949 | Addition complex and insertion isomers on the potential energy surface of the reaction of indium dimer with water studied with relativistic ECP. <i>Molecular Physics</i> , 2013, 111, 3025-3035. | 0.8 | 3 |
| 6950 | Silicon Acceleration of a Tandem Alkene Isomerization/Electrocyclic Ring-opening of 2-Methyleneoxetanes to α,β -Unsaturated Methylketones. <i>Journal of Organic Chemistry</i> , 2013, 78, 11213-11220. | 1.7 | 9 |
| 6951 | Accurate Computation of Cohesive Energies for Small to Medium-Sized Gold Clusters. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1964-1970. | 2.3 | 39 |
| 6952 | Accurate Surface Chemistry beyond the Generalized Gradient Approximation: Illustrations for Graphene Adatoms. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4853-4859. | 2.3 | 20 |
| 6953 | Electronic and magnetic properties of \pm -MnO from <i>ab initio</i> calculations. <i>Physical Review B</i> , 2013, 88, . | 1.1 | 46 |
| 6954 | Simulations of Acid Dissociation Constants of Polyprotic Acids in Near-Critical and Supercritical Water. <i>Journal of Physical Chemistry B</i> , 2013, 117, 15093-15100. | 1.2 | 3 |
| 6955 | Calculations of the Electric Fields in Liquid Solutions. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16236-16248. | 1.2 | 83 |
| 6956 | Effect of primary and secondary ligands on electronic structures and spectra of a series of nickel(II) complexes: a density functional theory study. <i>European Physical Journal D</i> , 2013, 67, 1. | 0.6 | 1 |
| 6957 | Molecular structure and vibrational spectral investigation of charge transfer NLO crystal Naphthalene Picrate for THz application. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 108, 256-267. | 2.0 | 19 |
| 6958 | Effect of Temperature and Substitution on Cope Rearrangement: A Symmetry Perspective. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12726-12733. | 1.1 | 13 |
| 6959 | Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 355-363. | 2.3 | 68 |
| 6960 | Two Rare-Class Tricyclic Diterpenes with Antitubercular Activity from the Caribbean Sponge <i>Svenzea flava</i> . Application of Vibrational Circular Dichroism Spectroscopy for Determining Absolute Configuration. <i>Journal of Organic Chemistry</i> , 2013, 78, 11294-11301. | 1.7 | 27 |
| 6961 | Redox Noninnocence in Coordinated 2-(Arylazo)pyridines: Steric Control of Ligand-Based Redox Processes in Cobalt Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 14040-14049. | 1.9 | 25 |
| 6962 | Triketramides A, Indole Alkaloids from the Australian Sponge <i>Triketron flabelliforme</i> . <i>Journal of Natural Products</i> , 2013, 76, 2100-2105. | 1.5 | 29 |
| 6963 | Reactions of molybdenum pentachloride with oxygen and nitrogen donor ligands. <i>Polyhedron</i> , 2013, 61, 188-194. | 1.0 | 17 |
| 6964 | Catalytic Mechanism and Allosteric Regulation of UDP-Glucose Pyrophosphorylase from <i>Leishmania major</i> . <i>ACS Catalysis</i> , 2013, 3, 2976-2985. | 5.5 | 25 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 6965 | Calculation of Heats of Formation for Zn Complexes: Comparison of Density Functional Theory, Second Order Perturbation Theory, Coupled-Cluster and Complete Active Space Methods. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5277-5285. | 2.3 | 23 |
| 6966 | All-Metal Aromaticity: Revisiting the Ring Current Model among Transition Metal Clusters. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4789-4796. | 2.3 | 90 |
| 6967 | Ground- and Excited-State Geometry Optimization of Small Organic Molecules with Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5513-5525. | 2.3 | 52 |
| 6968 | Coordination of Terpyridine to Li ⁺ in Two Different Ionic Liquids. <i>Inorganic Chemistry</i> , 2013, 52, 13167-13178. | 1.9 | 8 |
| 6969 | A simple monomer-based model-Hamiltonian approach to combine excitonic coupling and Jahn-Teller theory. <i>Journal of Chemical Physics</i> , 2013, 139, 174101. | 1.2 | 4 |
| 6970 | Oxidation of 1,3,2-diselenaphospholanes with an annelated dicarba-closo-dodecaborane(12) unit by addition of sulfur and selenium. Molecular structure of a novel 1,2,4,5-tetraselena-3-phospha heterocycle. <i>Journal of Organometallic Chemistry</i> , 2013, 747, 140-147. | 0.8 | 9 |
| 6971 | Theoretical Study of Nascent Solvation in Ni ⁺ (Benzene) _m , <i>m</i> = 3 and 4, Clusters. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12546-12559. | 1.1 | 10 |
| 6972 | Acylgermanes: Photoinitiators and Sources for Ge-Centered Radicals. Insights into their Reactivity. <i>Journal of the American Chemical Society</i> , 2013, 135, 17314-17321. | 6.6 | 95 |
| 6973 | [Cp ₂ TiCH ₂ CHMe(SiMe ₃) ⁺], an Alkyl-Titanium Complex Which (a) Exists in Equilibrium between a η^2 -Agostic and a Lower Energy η^3 -Agostic Isomer and (b) Undergoes Hydrogen Atom Exchange between η^2 -, η^2 -, and η^3 -Sites via a Combination of Conventional η^2 -Hydrogen Elimination-Reinsertion and a Nonconventional CH Bond Activation Process Which Involves Proton Tunnelling. <i>Journal of the American Chemical Society</i> , 2013, 135, 17514-17527. | 6.6 | 21 |
| 6974 | Brønsted Acid Catalyzed Enantioselective Indole Aza-Claisen Rearrangement Mediated by an Arene CH \cdots O Interaction. <i>Journal of the American Chemical Society</i> , 2013, 135, 16380-16383. | 6.6 | 80 |
| 6975 | Computation and Experiment Reveal That the Ring-Rearrangement Metathesis of Himbert Cycloadducts Can Be Subject to Kinetic or Thermodynamic Control. <i>Journal of the American Chemical Society</i> , 2013, 135, 17585-17594. | 6.6 | 27 |
| 6976 | Computational Studies on a Carbenoid Mechanism for the Doering-Moore-Skattebøl Reaction. <i>Journal of Organic Chemistry</i> , 2013, 78, 11815-11823. | 1.7 | 7 |
| 6977 | An amino acid coordinated vanadium (IV) complex: Synthesis, structure, DFT calculations and VHPO mimicking catalytic bromoperoxidation of organic substrates. <i>Inorganic Chemistry Communication</i> , 2013, 38, 43-46. | 1.8 | 31 |
| 6978 | Comparison of ReaxFF, DFTB, and DFT for Phenolic Pyrolysis. 2. Elementary Reaction Paths. <i>Journal of Physical Chemistry A</i> , 2013, 117, 11126-11135. | 1.1 | 41 |
| 6979 | Rational Design of Boradiazaindacene (BODIPY)-Based Functional Molecules. <i>Chemistry - A European Journal</i> , 2013, 19, 17766-17772. | 1.7 | 41 |
| 6980 | Behavior of Fluorescent Cholesterol Analogues Dehydroergosterol and Cholestatrienol in Lipid Bilayers: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5806-5819. | 1.2 | 32 |
| 6981 | Theoretical insight into electronic spectra of carbon chain carbenes H ₂ C _n (<i>n</i> = 3-10). <i>Journal of Chemical Physics</i> , 2013, 138, 204303. | 1.2 | 8 |
| 6982 | Hexamers and witchamers: Which hex do you choose?. <i>Computational and Theoretical Chemistry</i> , 2013, 1021, 70-83. | 1.1 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 6983 | Use of vibrational spectroscopy to study 2-[4-(N-dodecanoylamino)phenyl]-5-(4-nitrophenyl)-1,3,4-oxadiazole: A combined theoretical and experimental approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 114, 236-255. | 2.0 | 19 |
| 6984 | 5-Aminotetrazole induces spin crossover in iron(III) pentadentate Schiff base complexes: experimental and theoretical investigations. <i>Dalton Transactions</i> , 2013, 42, 16279. | 1.6 | 13 |
| 6985 | Homoleptic phosphorescent cyclometalated iridium(III) complexes with charge transporting groups: a theoretical study. <i>Molecular Simulation</i> , 2013, 39, 405-414. | 0.9 | 4 |
| 6986 | A chiral rhenium complex with predicted high parity violation effects: synthesis, stereochemical characterization by VCD spectroscopy and quantum chemical calculations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10952. | 1.3 | 21 |
| 6987 | Another Piece of the Membrane Puzzle: Extending Slipids Further. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 774-784. | 2.3 | 237 |
| 6988 | A comparative DFT study on aquation and nucleobase binding of ruthenium (II) and osmium (II) arene complexes. <i>Journal of Molecular Modeling</i> , 2013, 19, 4849-4856. | 0.8 | 5 |
| 6989 | Determining Adsorption Geometry, Bonding, and Translational Pathways of a Metal-Organic Complex on an Oxide Surface: Co-Salen on NiO(001). <i>Journal of Physical Chemistry C</i> , 2013, 117, 1105-1112. | 1.5 | 18 |
| 6990 | Strategies to Simultaneously Enhance the Hydrostability and the Alcohol-Water Separation Behavior of Cu-BTC. <i>Journal of Physical Chemistry C</i> , 2013, 117, 20706-20714. | 1.5 | 23 |
| 6991 | Redox-Linked Conformational Control of Proton-Coupled Electron Transfer: Y122 in the Ribonucleotide Reductase β 2 Subunit. <i>Journal of Physical Chemistry B</i> , 2013, 117, 8457-8468. | 1.2 | 18 |
| 6992 | Theoretical Analysis on the Kinetic Isotope Effects of Bimolecular Nucleophilic Substitution (SN2) Reactions and Their Temperature Dependence. <i>Molecules</i> , 2013, 18, 4816-4843. | 1.7 | 8 |
| 6993 | Stepwise magnetic behavior of the liquid crystal iron(III) complex. <i>Journal of Structural Chemistry</i> , 2013, 54, 16-27. | 0.3 | 7 |
| 6994 | Modeling continuous changes in substituent electronegativity and chemical hardness using fictitious nuclear potentials. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1. | 0.5 | 1 |
| 6995 | A scaling PNO-MP2 method using a hybrid OSV-PNO approach with an iterative direct generation of OSVs. <i>Molecular Physics</i> , 2013, 111, 2463-2476. | 0.8 | 60 |
| 6996 | Ruthenium carbonyl complexes of 3-(2-(methylthio)phenylazo)-4-hydroxy-3-penten-2-one: Synthesis, spectral characterization, electronic structure and catalytic activity. <i>Journal of Molecular Structure</i> , 2013, 1054-1055, 83-88. | 1.8 | 18 |
| 6997 | DFT study on reaction mechanisms of propylamine and dimethyl acetylenedicarboxylate with 1,3-dimethylalloxan. <i>Computational and Theoretical Chemistry</i> , 2013, 1004, 47-55. | 1.1 | 7 |
| 6998 | Reflectance anisotropy spectroscopy of Si(111)-(1x1) and Ag surfaces. <i>Physical Review B</i> , 2013, 87, . | 1.1 | 7 |
| 6999 | Tautomerism, Raman, infrared and ultraviolet-visible spectra, vibrational assignments, MP2 and B3LYP calculations of dienol 3,4-dihydropyridine, keto-enol 3-hydroxypyridin-4-one and keto-enol dimer. <i>Journal of Molecular Structure</i> , 2013, 1043, 52-67. | 1.8 | 7 |
| 7001 | Rhenium complexes of di-2-pyridyl ketone, 2-benzoylpyridine and 2-hydroxybenzophenone: A structural and theoretical study. <i>Polyhedron</i> , 2013, 62, 89-103. | 1.0 | 50 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7002 | Donor-Substituted Nitrocyclopropanes: Immediate Ring-Enlargement to Cyclic Nitronates. <i>Organic Letters</i> , 2013, 15, 6098-6101. | 2.4 | 73 |
| 7003 | Exploring the limits of redox non-innocence: pseudo square planar $[\{4\text{-Me}_2\text{C}(\text{CH}_2\text{N}(\text{CH}_2\text{py})_2)\text{Ni}\}]_n$ ($n = 2+$). <i>Tj ETQq</i> 1 0.784314 rg 3.7 27 | 3.7 | 27 |
| 7004 | C-($^2\text{-d}$ -Glucopyranosyl)formamidrazones, formic acid hydrazides and their transformations into 3-($^2\text{-d}$ -glucopyranosyl)-5-substituted-1,2,4-triazoles: a synthetic and computational study. <i>Tetrahedron</i> , 2013, 69, 10391-10404. | 1.0 | 24 |
| 7005 | Synthesis, reactivity and crystal structures of various solvates of fac-tris(trimethylphosphine)trichloroiridium. <i>Polyhedron</i> , 2013, 54, 67-73. | 1.0 | 7 |
| 7006 | Halogen effect on structure and ^{13}C NMR chemical shift of 3,6-disubstituted N -alkyl carbazoles. <i>Magnetic Resonance in Chemistry</i> , 2013, 51, 630-635. | 1.1 | 27 |
| 7007 | Effect of chemical modifications on the electronic structure of poly(3-hexylthiophene). <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2013, 51, 842-846. | 2.4 | 17 |
| 7008 | Modeling IR spectra of uranium monoxide clusters. <i>Journal of Applied Spectroscopy</i> , 2013, 80, 530-535. | 0.3 | 1 |
| 7009 | Simulation of nanodrug by theoretical approach. <i>Journal of Nanostructure in Chemistry</i> , 2013, 3, 1. | 5.3 | 18 |
| 7010 | Ab initio and anion photoelectron studies of Rh_n ($n = 1 \sim 9$) clusters. <i>European Physical Journal D</i> , 2013, 67, 1. | 0.6 | 31 |
| 7011 | Vibrational spectra and structure of borohydrides. <i>Journal of Alloys and Compounds</i> , 2013, 580, S122-S124. | 2.8 | 12 |
| 7012 | Crystal and molecular structure and electronic structure of a copper(II) complex with 10-(1-phthalazinylazo)-9-phenanthrol (HL) $[\text{Cu}_2(\text{L})_2(\text{H}_2\text{O})_4](\text{ClO}_4)_2$. <i>Russian Journal of Inorganic Chemistry</i> , 2013, 58, 1457-1464. | 0.3 | 3 |
| 7013 | The role of solvent exclusion in the interaction between D124 and the metal site in SOD1: implications for ALS. <i>Journal of Biological Inorganic Chemistry</i> , 2013, 18, 931-938. | 1.1 | 7 |
| 7014 | Theoretical study of oxygen contaminated silicon quantum dots: A case study for $\text{Si}_{29}\text{H}_{29}\text{xO}_{29}\text{y}$. <i>Microelectronic Engineering</i> , 2013, 112, 227-230. | 1.1 | 4 |
| 7015 | Toward extension of the gas-phase basicity scale by novel pyridine containing guanidines. <i>International Journal of Mass Spectrometry</i> , 2013, 354-355, 113-122. | 0.7 | 20 |
| 7016 | Substituent effects on the geometric and electronic properties of tetracyano- p -quinodimethane (TCNQ): a theoretical study. <i>Molecular Simulation</i> , 2013, 39, 350-356. | 0.9 | 5 |
| 7017 | First principles prediction of an insensitive high energy density material. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17681. | 1.3 | 18 |
| 7018 | Cation-Cation Interactions in $[(\text{UO}_2)_2(\text{OH})_n]^{2+n+}$ Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 11269-11279. | 1.9 | 8 |
| 7019 | Spectroscopic properties of N_1, N_5 -bis[pyridine-2-methylene]-thiocarbohydrazone and its corresponding zinc (II) and nickel (II) metal complexes: A DFT and TD-DFT study. <i>Synthetic Metals</i> , 2013, 175, 174-182. | 2.1 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7021 | Ab Initio Calculation of Molecular Aggregation Effects: A Coumarin-343 Case Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 11072-11085. | 1.1 | 15 |
| 7022 | Toward Reliable Prediction of the Energy Ladder in Multichromophoric Systems: A Benchmark Study on the FMO Light-Harvesting Complex. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4928-4938. | 2.3 | 52 |
| 7023 | Proton transfer or hemibonding? The structure and stability of radical cation clusters. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16214. | 1.3 | 39 |
| 7024 | Effects of the Protein Environment on the Spectral Properties of Tryptophan Radicals in <i>Pseudomonas aeruginosa</i> Azurin. <i>Journal of the American Chemical Society</i> , 2013, 135, 4822-4833. | 6.6 | 26 |
| 7025 | A Complete Guide on the Influence of Metal Clusters in the Diels-Alder Regioselectivity of C_{80} Endohedral Metallofullerenes. <i>Chemistry - A European Journal</i> , 2013, 19, 14931-14940. | 1.7 | 37 |
| 7026 | 8-Quinolinolate complexes of yttrium and ytterbium: molecular arrangement and fragmentation under laser impact. <i>Dalton Transactions</i> , 2013, 42, 15699. | 1.6 | 27 |
| 7027 | Role of Metal Ion in Specific Recognition of Pyrophosphate Ion under Physiological Conditions and Hydrolysis of the Phosphoester Linkage by Alkaline Phosphatase. <i>Inorganic Chemistry</i> , 2013, 52, 11034-11041. | 1.9 | 60 |
| 7028 | A density functional theory study of the reactivity descriptors and antioxidant behavior of Crocin. <i>Computational and Theoretical Chemistry</i> , 2013, 1013, 123-129. | 1.1 | 44 |
| 7029 | Structures and optical absorptions of PbSe clusters from <i>ab initio</i> calculations. <i>Journal of Chemical Physics</i> , 2013, 139, 094305. | 1.2 | 16 |
| 7030 | Discovery of Most Stable Structures of Neutral and Anionic Phenylalanine through Automated Scanning of Tautomeric and Conformational Spaces. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4374-4381. | 2.3 | 5 |
| 7031 | Theoretical Study of Spin-State and Redox Multistability in an Iron [2+2] Grid Complex. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 1009-1014. | 1.0 | 16 |
| 7032 | Electron correlation and relativistic effects in the secondary NMR isotope shifts of CSe ₂ . <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17468. | 1.3 | 6 |
| 7033 | Formation of S-Cl Phosphorothioate Adduct Radicals in dsDNA S-Oligomers: Hole Transfer to Guanine vs Disulfide Anion Radical Formation. <i>Journal of the American Chemical Society</i> , 2013, 135, 12827-12838. | 6.6 | 27 |
| 7034 | Synthesis and Characterization of Heterobimetallic (Pd/B) Nindigo Complexes and Comparisons to Their Homobimetallic (Pd ₂ , B ₂) Analogues. <i>Inorganic Chemistry</i> , 2013, 52, 10912-10919. | 1.9 | 16 |
| 7035 | Solid state NMR studies and chemical shift calculations of a gold(I) complex with a diphosphacyclobutadiene cobaltate sandwich anion. <i>Solid State Nuclear Magnetic Resonance</i> , 2013, 53, 13-19. | 1.5 | 10 |
| 7036 | From Bis(silylene) and Bis(germylene) Pincer-Type Nickel(II) Complexes to Isolable Intermediates of the Nickel-Catalyzed Sonogashira Cross-Coupling Reaction. <i>Journal of the American Chemical Society</i> , 2013, 135, 15617-15626. | 6.6 | 232 |
| 7037 | Theoretical Study on the Conformation and Aromaticity of Regular and Singly N-Confused [28]Hexaphyrins. <i>Journal of Organic Chemistry</i> , 2013, 78, 9317-9327. | 1.7 | 22 |
| 7038 | Nuclear spin-induced Cotton-Mouton effect in molecules. <i>Journal of Chemical Physics</i> , 2013, 138, 204110. | 1.2 | 19 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7039 | Atmospheric Significance of Water Clusters and Ozone-Water Complexes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10381-10396. | 1.1 | 101 |
| 7040 | Stereocontrolled Cyanohydrin Ether Synthesis through Chiral Brønsted Acid-Mediated Vinyl Ether Hydrocyanation. <i>Journal of Organic Chemistry</i> , 2013, 78, 9366-9376. | 1.7 | 26 |
| 7041 | Tautomers and UV-Induced Photoisomerization of a Strongly Intramolecularly H-Bonded Aromatic Azo-Dye: 1-(Cyclopropyl)diazo-2-naphthol. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10671-10680. | 1.1 | 21 |
| 7042 | Oxidative Decomposition of Propylene Carbonate in Lithium Ion Batteries: A DFT Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7959-7969. | 1.1 | 28 |
| 7043 | Molecular Dynamics Simulations of Graphene Oxide Frameworks. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4890-4900. | 2.3 | 35 |
| 7044 | The prototropic tautomerism and substituent effect through strong electron-withdrawing group in (E)-5-(diethylamino)-2-[(3-nitrophenylimino)methyl]phenol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 114, 205-213. | 2.0 | 20 |
| 7045 | Synthesis and Structure of a Trinuclear Pd-Ag-Pd Carbene Acetato Complex. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2013, 639, 1237-1241. | 0.6 | 5 |
| 7046 | Mechanistic Basis for High Stereoselectivity and Broad Substrate Scope in the (salen)Co(III)-Catalyzed Hydrolytic Kinetic Resolution. <i>Journal of the American Chemical Society</i> , 2013, 135, 15595-15608. | 6.6 | 115 |
| 7047 | Geometries and Vertical Excitation Energies in Retinal Analogues Resolved at the CASPT2 Level of Theory: Critical Assessment of the Performance of CASSCF, CC2, and DFT Methods. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4915-4927. | 2.3 | 26 |
| 7048 | Theoretical and Experimental Analysis of the Reaction Mechanism of MrTPS2, a Triquinane-Forming Sesquiterpene Synthase from Chamomile. <i>Chemistry - A European Journal</i> , 2013, 19, 13590-13600. | 1.7 | 30 |
| 7049 | Crystal and electronic structures of tris[4,4,4-Trifluoro-1-(2-X)-1,3-butanedionato]iron(III) isomers (X=thienyl or furyl): An X-ray and computational study. <i>Journal of Molecular Structure</i> , 2013, 1053, 134-140. | 1.8 | 21 |
| 7050 | Recoil Effects in Valence Band Photoemission of Organic Solids. <i>Analytical Chemistry</i> , 2013, 85, 3739-3745. | 3.2 | 4 |
| 7051 | Red-Hair-Inspired Chromogenic System Based on a Proton-Switched Dehydrogenative Free-Radical Coupling. <i>Organic Letters</i> , 2013, 15, 4944-4947. | 2.4 | 14 |
| 7052 | Implementation of the CCSD-PCM linear response function for frequency dependent properties in solution: Application to polarizability and specific rotation. <i>Journal of Chemical Physics</i> , 2013, 139, 114103. | 1.2 | 29 |
| 7053 | Mechanistic Investigations into the Enantioselective Conia-Ene Reaction Catalyzed by Cinchona-Derived Amino Urea Pre-Catalysts and Cu(I). <i>Chemistry - A European Journal</i> , 2013, 19, 14286-14295. | 1.7 | 30 |
| 7054 | A comparison between state-specific and linear-response formalisms for the calculation of vertical electronic transition energy in solution with the CCSD-PCM method. <i>Journal of Chemical Physics</i> , 2013, 139, 044116. | 1.2 | 61 |
| 7055 | Double-hybrid density functionals: merging wavefunction and density approaches to get the best of both worlds. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14581. | 1.3 | 100 |
| 7056 | Complexes of Cu(I) with nitroxides and their magnetochemical behavior. <i>Russian Chemical Bulletin</i> , 2013, 62, 2337-2344. | 0.4 | 6 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7057 | Adsorption of S ²⁻ and HS ⁻ ions on the (111) face of coinage metals: A quantum-chemical study. Russian Journal of Electrochemistry, 2013, 49, 1031-1038. | 0.3 | 2 |
| 7058 | Molecular anions of uranium fluorides and oxides: First principle based relativistic calculations. Radiochemistry, 2013, 55, 353-356. | 0.2 | 10 |
| 7059 | Synthesis, structure, and properties of a new phosphorus-containing Schiff's base, a derivative of pyrazole-5-one. Russian Journal of General Chemistry, 2013, 83, 1376-1382. | 0.3 | 5 |
| 7060 | Transition metal complexes with 2,6-Di-tert-butyl-p-quinone 1 ² -phthalazinyldiazine. Russian Journal of General Chemistry, 2013, 83, 1928-1936. | 0.3 | 5 |
| 7061 | On the existence of oxide molecules of plutonium in highest oxidation states. Doklady Chemistry, 2013, 448, 1-3. | 0.2 | 17 |
| 7062 | DFT study of the mechanism for methane hydroxylation by soluble methane monooxygenase (sMMO): effects of oxidation state, spin state, and coordination number. Dalton Transactions, 2013, 42, 1011-1023. | 1.6 | 40 |
| 7063 | Differences between polymer/salt and single ion conductor solid polymer electrolytes. RSC Advances, 2013, 3, 1564-1571. | 1.7 | 44 |
| 7064 | Fluorescent unsymmetrical four-ring bent-core mesogens: 2D modulated phases. CrystEngComm, 2013, 15, 10510. | 1.3 | 10 |
| 7065 | Hetero triply-bridged dinuclear copper ($\langle \text{scp} \rangle \text{ii} \langle / \text{scp} \rangle$) compounds with ferromagnetic coupling: a challenge for current density functionals. Physical Chemistry Chemical Physics, 2013, 15, 1966-1975. | 1.3 | 21 |
| 7066 | C-H...N interactions as modulators of carbocation structure - implications for terpene biosynthesis. Chemical Science, 2013, 4, 2512. | 3.7 | 45 |
| 7067 | On the Acceleration of Cu Electrodeposition by TBPS (3,3-thiobis-1-propanesulfonic acid): A Combined Electrochemical, STM, NMR, ESI-MS and DFT Study. Journal of the Electrochemical Society, 2013, 160, D3158-D3164. | 1.3 | 18 |
| 7068 | π -Alkylidene Complexes of Rhodium(I) and Iridium(I): Their Reactivity with Dioxygen and Dihydrogen. European Journal of Inorganic Chemistry, 2013, 2013, 4775-4788. | 1.0 | 7 |
| 7069 | Clarification of the role of protein in carbonmonoxy myoglobin by investigating electronic states. International Journal of Quantum Chemistry, 2013, 113, 2345-2354. | 1.0 | 5 |
| 7070 | Dispersion Corrected Hartree-Fock and Density Functional Theory for Organic Crystal Structure Prediction. Topics in Current Chemistry, 2013, 345, 1-23. | 4.0 | 72 |
| 7071 | Diperoxo Peractinetic Acid Characterized by Spectroscopic and Quantum Chemical Studies. European Journal of Inorganic Chemistry, 2013, 2013, 4595-4600. | 1.0 | 5 |
| 7072 | Copper(II)-imidazole-salen Complexes Encapsulated into NaY Zeolite for Oxidations Reactions. European Journal of Inorganic Chemistry, 2013, 2013, 5408-5417. | 1.0 | 14 |
| 7073 | Intramolecular CH...N interactions in alkylaromatics: Monomer conformations for poly(3-alkylthiophene) atomistic models. International Journal of Quantum Chemistry, 2013, 113, 2154-2162. | 1.0 | 31 |
| 7074 | A microiterative intrinsic reaction coordinate method for large QM/MM systems. Physical Chemistry Chemical Physics, 2013, 15, 14188. | 1.3 | 10 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7075 | Autocatalytic cathodic dehalogenation triggered by dissociative electron transfer through a C-H \cdots O hydrogen bond. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17522. | 1.3 | 9 |
| 7076 | Probing the valence orbitals of transition metal σ -silicon diatomic anions: ZrSi, NbSi, MoSi, PdSi and WSi. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6068. | 1.3 | 23 |
| 7077 | A simple and rapid route to novel tetra(4-thiaalkyl)ammonium bromides. <i>RSC Advances</i> , 2013, 3, 24612. | 1.7 | 11 |
| 7078 | Computational Hammett analysis of redox based oxy-insertion by Pt(σ) complexes. <i>Dalton Transactions</i> , 2013, 42, 4114-4121. | 1.6 | 4 |
| 7079 | Theoretical study on low-lying states of Ga ₂ X (X = P, As) with coupled-cluster approaches. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17929. | 1.3 | 1 |
| 7080 | Bisactinyl halogenated complexes: relativistic density functional theory calculation and experimental synthesis. <i>RSC Advances</i> , 2013, 3, 1572-1582. | 1.7 | 8 |
| 7081 | Theoretical study of heavy-atom tuning of nonlinear optical properties in group 15 derivatives of N,N,N-trimethylglycine (betaine). <i>Dalton Transactions</i> , 2013, 42, 3695. | 1.6 | 4 |
| 7082 | Change in energy of hydrogen bonds upon excitation of 6-aminocoumarin: TDDFT/EFP1 study. <i>New Journal of Chemistry</i> , 2013, 37, 2648. | 1.4 | 11 |
| 7083 | Reaction time dependent formation of Pd(σ) and Pt(σ) complexes of bis(methyl)thiasalen podand. <i>Dalton Transactions</i> , 2013, 42, 476-483. | 1.6 | 12 |
| 7084 | Activation of Si σ -Si and Si σ -H bonds at Pt: a catalytic hydrogenolysis of silicon σ -silicon bonds. <i>Dalton Transactions</i> , 2013, 42, 4052. | 1.6 | 21 |
| 7085 | Synthesis of dithienosilole-based highly photoluminescent donor π -acceptor type compounds. <i>Dalton Transactions</i> , 2013, 42, 3646. | 1.6 | 19 |
| 7086 | Staying hydrated: the molecular journey of gaseous sulfur dioxide to a water surface. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6893. | 1.3 | 17 |
| 7087 | Flavans from <i>Desmos cochinchinensis</i> as potent aromatase inhibitors. <i>MedChemComm</i> , 2013, 4, 1590. | 3.5 | 8 |
| 7088 | Asymmetric niobium guanidates as intermediates in the catalytic guanylation of amines. <i>Dalton Transactions</i> , 2013, 42, 8223. | 1.6 | 28 |
| 7089 | Photoinduced Nonadiabatic Decay and Dissociation Dynamics of Dimethylnitramine. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4785-4793. | 1.1 | 11 |
| 7090 | Pseudo-symmetry Analysis of the d-block Molecular Orbitals in Four-Coordinate Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 6510-6519. | 1.9 | 8 |
| 7091 | Molecular Structures for FeS ₄ ⁰ As Determined from an ab Initio Study of the Anion Photoelectron Spectra. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3227-3234. | 1.1 | 14 |
| 7092 | Wagging the Tail: Essential Role of Substrate Flexibility in FAAH Catalysis. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1202-1213. | 2.3 | 24 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7093 | On the method-dependence of transition state asynchronicity in Diels-Alder reactions. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5108. | 1.3 | 76 |
| 7094 | Highly efficient SO ₂ capture through tuning the interaction between anion-functionalized ionic liquids and SO ₂ . <i>Chemical Communications</i> , 2013, 49, 1166-1168. | 2.2 | 114 |
| 7095 | Reaction pathways and free energy profiles for spontaneous hydrolysis of urea and tetramethylurea: unexpected substituent effects. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 7595. | 1.5 | 21 |
| 7096 | Diverse bonding modes of the tetramethyleneethane ligand in binuclear iron carbonyl derivatives. <i>New Journal of Chemistry</i> , 2013, 37, 709-716. | 1.4 | 1 |
| 7097 | Topological control in radical reactions of cholesterol in model dyads. <i>Chemical Science</i> , 2013, 4, 1608. | 3.7 | 17 |
| 7098 | Oxidation state and covalency in f-element metallocenes (M = Ce, Th, Pu): a combined CASSCF and topological study. <i>Dalton Transactions</i> , 2013, 42, 16428. | 1.6 | 90 |
| 7099 | Syntheses and structures of eight-semi-coordinate M(II) (M=Mn, Fe, Co, Ni, Cu, Zn) complexes and density functional theory study of bond dissociation energies for the MO semi coordinate bonds. <i>Inorganic Chemistry Communication</i> , 2013, 27, 114-118. | 1.8 | 8 |
| 7100 | Consistent descriptions of metal-ligand bonds and spin-crossover in inorganic chemistry. <i>Coordination Chemistry Reviews</i> , 2013, 257, 196-209. | 9.5 | 172 |
| 7101 | Interaction of aromatic alcohols, aldehydes and acids with $\dot{\text{I}}\text{-hydroxyl}$ -containing carbon-centered radicals: A steady state radiolysis study. <i>Radiation Physics and Chemistry</i> , 2013, 82, 35-43. | 1.4 | 7 |
| 7102 | Surface-enhanced Raman scattering study of the adsorption of croconate violet on colloidal silver particles. <i>Vibrational Spectroscopy</i> , 2013, 64, 153-157. | 1.2 | 5 |
| 7103 | Density functional theory studies on the structure, spectra (FT-IR, FT-Raman, and UV) and first order molecular hyperpolarizability of 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine: Comparison to experimental data. <i>Vibrational Spectroscopy</i> , 2013, 64, 134-147. | 1.2 | 45 |
| 7104 | Evidence of $\pi\text{-}\pi$ stacking interactions in the self-assembly of hIAPP ₂₂₋₂₉ . <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 690-703. | 1.5 | 43 |
| 7105 | Mechanisms for the Formation of Acenes from $\dot{\text{I}}\text{-Diketones}$ by Bisdecarbonylation. <i>Journal of Organic Chemistry</i> , 2013, 78, 1851-1857. | 1.7 | 18 |
| 7106 | A Systematic Approach to Identify Cooperatively Bound Homotrimers. <i>Journal of Physical Chemistry A</i> , 2013, 117, 174-182. | 1.1 | 18 |
| 7107 | Quantum chemical study of the catalytic activation of methane by copper oxide and copper hydroxide cations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 1148-1153. | 1.3 | 16 |
| 7108 | Benchmarking the Starting Points of the <i>GW</i> Approximation for Molecules. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 324-329. | 2.3 | 206 |
| 7109 | Solvent effects on ¹⁵ N NMR coordination shifts. <i>Magnetic Resonance in Chemistry</i> , 2013, 51, 46-53. | 1.1 | 28 |
| 7110 | Quantum-Mechanical Analysis of the Energetic Contributions to π Stacking in Nucleic Acids versus Rise, Twist, and Slide. <i>Journal of the American Chemical Society</i> , 2013, 135, 1306-1316. | 6.6 | 80 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7111 | A mass spectrometric investigation of clusters formed by sodium cations and pentacyanonitrosylferrate(2a^{3-}) anions in the gas phase, and an exploration of structures of some of the clusters using Density Functional Theory. <i>Inorganica Chimica Acta</i> , 2013, 394, 300-309. | 1.2 | 2 |
| 7112 | Metal-Free Benzodithiophene-Containing Organic Dyes for Dye-Sensitized Solar Cells. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 84-94. | 1.2 | 36 |
| 7113 | Structural phase transitions of the metal oxide perovskites SrTiO_3 , LaAlO_3 , and LaTiO_3 . <i>Journal of Chemical Physics</i> , 2013, 138, 024111. | 1.1 | 51 |
| 7114 | A Candidate Ion-Retaining State in the Inward-Facing Conformation of Sodium/Galactose Symporter: Clues from Atomistic Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1240-1246. | 2.3 | 26 |
| 7115 | Benchmarking density-functional theory calculations of NMR shielding constants and spin-rotation constants using accurate coupled-cluster calculations. <i>Journal of Chemical Physics</i> , 2013, 138, 024111. | 1.2 | 153 |
| 7116 | Dynamic Behavior of Hydrogen in Transition Metal Bis(silyl) Hydride Complexes. <i>Organometallics</i> , 2013, 32, 514-526. | 1.1 | 7 |
| 7117 | Mechanistic Studies on the Roles of the Oxidant and Hydrogen Bonding in Determining the Selectivity in Alkene Oxidation in the Presence of Molybdenum Catalysts. <i>Chemistry - A European Journal</i> , 2013, 19, 2030-2040. | 1.7 | 14 |
| 7118 | Electronic structure tuning of diamondoids through functionalization. <i>Journal of Chemical Physics</i> , 2013, 138, 024310. | 1.2 | 51 |
| 7119 | Polarized Molecular Orbital Model Chemistry 3. The PMO Method Extended to Organic Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 33-45. | 2.3 | 18 |
| 7120 | Generalized Born Solvation Model SM12. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 609-620. | 2.3 | 170 |
| 7121 | The Precise Chemical-Physical Nature of the Pharmacore in FK506 Binding Protein Inhibition: ElteX, a New Class of Nanomolar FKBP12 Ligands. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 1041-1051. | 2.9 | 28 |
| 7122 | A Heterobimetallic Approach To Stabilize the Elusive Disulfur Radical Trianion (S_2^{3-}). <i>Chemistry - A European Journal</i> , 2013, 19, 1246-1253. | 1.7 | 9 |
| 7123 | A Critical Assessment of Two-Body and Three-Body Interactions in Water. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1103-1114. | 2.3 | 126 |
| 7124 | Theoretical investigation on Pt- and Au-mediated cycloisomerizations of propargylic 3-indoleacetate: [3 + 2]- versus [2 + 2]-cycloaddition products. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 336-343. | 1.5 | 17 |
| 7125 | Bond-strengthening backdonation in a transition-metal π -diborene complex. <i>Nature Chemistry</i> , 2013, 5, 115-121. | 6.6 | 137 |
| 7126 | Ring opening polymerization of rac-lactide by group 4 tetracarbamato complexes: activation, propagation and role of the metal. <i>Dalton Transactions</i> , 2013, 42, 2792-2802. | 1.6 | 33 |
| 7127 | Adsorption characteristics of 1,2,4-trichlorobenzene, 2,4,6-trichlorophenol, 2-naphthol and naphthalene on graphene and graphene oxide. <i>Carbon</i> , 2013, 51, 156-163. | 5.4 | 311 |
| 7128 | Pyrazolium- versus Imidazolium-Based Ionic Liquids: Structure, Dynamics and Physicochemical Properties. <i>Journal of Physical Chemistry B</i> , 2013, 117, 668-676. | 1.2 | 49 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7129 | Combined theoretical and experimental study on the molecular structure, FT-IR, and NMR spectra of cyadox and 1,4-bisdesoxycyadox. <i>Journal of Molecular Structure</i> , 2013, 1035, 69-75. | 1.8 | 3 |
| 7130 | Cluster-Continuum Calculations of Hydration Free Energies of Anions and Group 12 Divalent Cations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 555-569. | 2.3 | 44 |
| 7131 | Interfacial States in Donor-Acceptor Organic Heterojunctions: Computational Insights into Thiophene-Oligomer/Fullerene Junctions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 533-542. | 2.3 | 45 |
| 7132 | N ⁺ As intramolecularly coordinated organoarsenic(III) chalcogenides: Isolation of terminal As-S and As-Se bonds. <i>Journal of Organometallic Chemistry</i> , 2013, 723, 10-14. | 0.8 | 8 |
| 7133 | General treatment of the multimode Jahn-Teller effect: study of fullerene cations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 1252-1259. | 1.3 | 20 |
| 7134 | Parametrization and Benchmark of DFTB3 for Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 338-354. | 2.3 | 743 |
| 7135 | Chain-Amplified Photochemical Fragmentation of <i>N</i> -Alkoxy pyridinium Salts: Proposed Reaction of Alkoxy Radicals with Pyridine Bases To Give Pyridinyl Radicals. <i>Journal of Organic Chemistry</i> , 2013, 78, 1955-1964. | 1.7 | 21 |
| 7136 | Synthesis, structure, magnetic properties and theoretical calculations of methoxy bridged dinuclear iron(III) complex with hydrazone based O,N,N-donor ligand. <i>Dalton Transactions</i> , 2013, 42, 2803-2812. | 1.6 | 38 |
| 7137 | Long-Range Corrected Hybrid Density Functionals with Improved Dispersion Corrections. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 263-272. | 2.3 | 535 |
| 7138 | Dependence of the optical absorption and Na ⁺ binding energies of coumarin-crown ethers on the size and attachment position of ether ring: density functional investigation. <i>Journal of Molecular Modeling</i> , 2013, 19, 173-178. | 0.8 | 3 |
| 7139 | Prodrugs of fumarate esters for the treatment of psoriasis and multiple sclerosis—a computational approach. <i>Journal of Molecular Modeling</i> , 2013, 19, 439-452. | 0.8 | 15 |
| 7140 | 5-[4-(Dimethylamino)phenyl]-2-benzamidopyrazines: fluorescent dyes based on Cypridina oxyluciferin. <i>Research on Chemical Intermediates</i> , 2013, 39, 233-245. | 1.3 | 9 |
| 7141 | Lowest triplet (<i>n</i> , π^*) electronic state of acrolein: Determination of structural parameters by cavity ringdown spectroscopy and quantum-chemical methods. <i>Journal of Chemical Physics</i> , 2013, 138, 064303. | 1.2 | 6 |
| 7142 | Small clusters of formic acid: Tests and applications of density functional theory with dispersion-correcting potentials. <i>Chemical Physics Letters</i> , 2013, 560, 71-74. | 1.2 | 14 |
| 7143 | Analysis of UV and vibrational spectra (FT-IR and FT-Raman) of hexachlorocyclotriphosphazene based on normal coordinate analysis, MP2 and DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 105, 446-455. | 2.0 | 9 |
| 7144 | Molecular structure, Normal Coordinate Analysis, harmonic vibrational frequencies, Natural Bond Orbital, TD-DFT calculations and biological activity analysis of antioxidant drug 7-hydroxycoumarin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 101, 370-381. | 2.0 | 23 |
| 7145 | A 3D supramolecular network assembly based on thiacalix[4]arene by halogen-halogen, C-H \cdots Br, C-H \cdots I, and S \cdots I interactions. <i>Tetrahedron Letters</i> , 2013, 54, 1510-1514. | 0.7 | 21 |
| 7146 | Implicit inclusion of atomic polarization in modeling of partitioning between water and lipid bilayers. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4677. | 1.3 | 43 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7147 | Understanding Pd–Pd Bond Length Variation in (PNP)Pd–Pd(PNP) Dimers. <i>Inorganic Chemistry</i> , 2013, 52, 2317-2322. | 1.9 | 15 |
| 7148 | Understanding the Adsorption Mechanism of C ₂ H ₂ , CO ₂ , and CH ₄ in Isostructural Metal–Organic Frameworks with Coordinatively Unsaturated Metal Sites. <i>Journal of Physical Chemistry C</i> , 2013, 117, 2824-2834. | 1.5 | 92 |
| 7149 | Double oxidation localizes spin in a Ni bis-phenoxy radical complex. <i>Dalton Transactions</i> , 2013, 42, 3950. | 1.6 | 31 |
| 7151 | Cross–Hyperconjugation: An Unexplored Orbital Interaction between π -Conjugated and Saturated Molecular Segments. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 983-987. | 7.2 | 35 |
| 7152 | The Effect of Stereochemistry on the Biological Activity of Natural Phytotoxins, Fungicides, Insecticides and Herbicides. <i>Chirality</i> , 2013, 25, 59-78. | 1.3 | 44 |
| 7153 | An efficient method for calculating dynamical hyperpolarizabilities using real-time time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2013, 138, 064104. | 1.2 | 72 |
| 7154 | Calculating excited state properties using Kohn-Sham density functional theory. <i>Journal of Chemical Physics</i> , 2013, 138, 064101. | 1.2 | 47 |
| 7155 | Electrochemical study of carbonyl phosphine η^2 -diketonato rhodium(I) complexes. <i>Electrochimica Acta</i> , 2013, 113, 519-526. | 2.6 | 15 |
| 7156 | Theoretical studies on acetylene cyclotrimerization into benzene catalyzed by Cp^*Ir fragment. <i>Journal of Organometallic Chemistry</i> , 2013, 748, 29-35. | 0.8 | 24 |
| 7157 | Theoretical study on copper-catalyzed reaction of hydrosilane, alkyne and carbon dioxide: A hydrocarboxylation or a hydrosilylation process?. <i>Journal of Organometallic Chemistry</i> , 2013, 745-746, 166-172. | 0.8 | 13 |
| 7158 | Fragmentation reactions of Si ₂ Cl ₆ ⁺ in the gas phase—A quantum-chemical and mass-spectrometric assessment. <i>International Journal of Mass Spectrometry</i> , 2013, 354-355, 378-390. | 0.7 | 5 |
| 7159 | Ionization/dissociation processes of methyl-substituted derivatives of cyclopentanone in intense femtosecond laser field. <i>Chemical Physics Letters</i> , 2013, 586, 21-28. | 1.2 | 10 |
| 7160 | On the formation of naphthalene cation in space from small hydrocarbon molecules: A theoretical study. <i>Chemical Physics Letters</i> , 2013, 564, 11-15. | 1.2 | 6 |
| 7161 | Experimental and theoretical investigations on the tautomerism of 1-phenyl-2-thiobarbituric acid and its methylation reaction. <i>Journal of Molecular Structure</i> , 2013, 1036, 372-379. | 1.8 | 4 |
| 7162 | Biological activity of Pd(II) complexes with mono- and disubstituted pyridines—Experimental and theoretical studies. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 2765-2768. | 1.0 | 7 |
| 7163 | Synthesis, crystal structure and DFT analysis of a phenoxo bridged Cu(II) complex and an azide and μ_3 -O mixed bridged trinuclear Cu(II) complex. <i>Polyhedron</i> , 2013, 50, 51-58. | 1.0 | 15 |
| 7164 | Tetragonally compressed high-spin Mn(III) Schiff base complex: Synthesis, crystal structure, magnetic properties and theoretical calculations. <i>Polyhedron</i> , 2013, 52, 1199-1205. | 1.0 | 22 |
| 7165 | Synthesis, spectroscopic, thermal and quantum chemical studies on trivalent erbium NO chelating sulfamonomethoxine–cyclophosph(V)azane complex. <i>Journal of Molecular Structure</i> , 2013, 1048, 202-209. | 1.8 | 2 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7166 | Unusual solvent dependent emission property of two new ruthenium(II) complexes. <i>Inorganica Chimica Acta</i> , 2013, 402, 75-82. | 1.2 | 10 |
| 7167 | The mechanism of addition of aldehydes to germene in different solvents: A DFT study. <i>Journal of Organometallic Chemistry</i> , 2013, 748, 8-12. | 0.8 | 4 |
| 7168 | Synthesis of hafnium(IV) η^2 -ketoiminates as potential precursors for the MOCVD of HfO ₂ . <i>Inorganica Chimica Acta</i> , 2013, 396, 60-65. | 1.2 | 3 |
| 7169 | Theoretical study on the CH \cdots NC hydrogen bond interaction in thiophene-based molecules. <i>Computational and Theoretical Chemistry</i> , 2013, 1005, 45-52. | 1.1 | 5 |
| 7170 | Synthesis, growth and spectral studies of S-benzyl isothiuronium nitrate by density functional methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 109, 1-7. | 2.0 | 5 |
| 7171 | Path Length Determines the Tunneling Decay of Substituted Carbenes. <i>Chemistry - A European Journal</i> , 2013, 19, 8207-8212. | 1.7 | 38 |
| 7172 | New Diruthenium Bis-alkynyl Compounds as Potential Ditopic Linkers. <i>Organometallics</i> , 2013, 32, 6461-6467. | 1.1 | 5 |
| 7173 | Assessment of Density Functional Theory for Thermochemical Approaches Based on Bond Separation Reactions. <i>Journal of Physical Chemistry A</i> , 2013, 117, 228-243. | 1.1 | 16 |
| 7174 | Interaction between the Cesium Cation and Cesium Carboxylates: An Extended Cs ⁺ Basicity Scale. <i>ChemPlusChem</i> , 2013, 78, 1195-1204. | 1.3 | 7 |
| 7175 | Dicyclopalladated Complexes of Asymmetrically Substituted Azobenzenes: Synthesis, Kinetics and Mechanisms. <i>Inorganic Chemistry</i> , 2013, 52, 12749-12757. | 1.9 | 21 |
| 7176 | Static and Field-Oriented Properties of Bowl-Shaped Polynuclear Aromatic Hydrocarbon Fragments. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4797-4804. | 2.3 | 12 |
| 7177 | Bifunctional mesoporous MCF materials as catalysts in the FriedlÄnder condensation. <i>Catalysis Today</i> , 2013, 218-219, 70-75. | 2.2 | 23 |
| 7178 | Mechanism and Substrate-Dependent Rate-Determining Step in Palladium-Catalyzed Intramolecular Decarboxylative Coupling of Arenecarboxylic Acids with Aryl Bromides: A DFT Study. <i>Organometallics</i> , 2013, 32, 6957-6968. | 1.1 | 21 |
| 7179 | Investigation of (m=2-5, n=2-3) clusters using photoelectron spectroscopy and density functional calculations. <i>Chemical Physics Letters</i> , 2013, 564, 6-10. | 1.2 | 2 |
| 7180 | Experimental and theoretical approaches for identification of p-benzophenoneoxycarbonylphenyl acrylate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 113, 80-91. | 2.0 | 15 |
| 7181 | Light emitting mechanisms in an alternated fluorene EDOT copolymerâ€”A theoretical and photophysical study. <i>Journal of Luminescence</i> , 2013, 134, 670-677. | 1.5 | 7 |
| 7182 | Raman scattering from 1,3-propanedithiol at a hot spot: Theory meets experiment. <i>Chemical Physics Letters</i> , 2013, 581, 57-63. | 1.2 | 16 |
| 7183 | Theoretical insight into the mechanism of Pt(η^3 -allyl)-catalyzed [3+2] cycloaddition reactions of propadienyl silyl ethers with alkenyl ethers. <i>Journal of Organometallic Chemistry</i> , 2013, 724, 192-199. | 0.8 | 2 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7184 | Methyl-to-double bond transfer in the gas phase: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2013, 1020, 7-13. | 1.1 | 0 |
| 7185 | Adsorption of a single Pt atom on polyaromatic hydrocarbons from first-principle calculations. <i>Chemical Physics Letters</i> , 2013, 575, 76-80. | 1.2 | 8 |
| 7186 | Prediction of the emission wavelengths of metal-organic triplet emitters by quantum chemical calculations. <i>Journal of Organometallic Chemistry</i> , 2013, 748, 63-67. | 0.8 | 18 |
| 7187 | Nematic phases in achiral unsymmetrical four-ring bent-core azo compounds possessing strongly polar cyano and nitro moieties as end substituents: Synthesis and characterization. <i>Dyes and Pigments</i> , 2013, 99, 447-455. | 2.0 | 26 |
| 7188 | Magnetolectric effect in organometallic vanadium benzene wires. <i>Chemical Physics Letters</i> , 2013, 568-569, 121-124. | 1.2 | 10 |
| 7189 | Reductive debromination of decabromodiphenyl ether yields brominated dibenzofurans in a Pschorr-type cyclisation. <i>Electrochemistry Communications</i> , 2013, 37, 64-67. | 2.3 | 7 |
| 7190 | Use of a Ru/Os-CO-diiodide precursor to synthesize heteroleptic 1-alkyl-2-(aryloxy)imidazole complexes: The structural characterization, electrochemistry and catalytic activity. <i>Polyhedron</i> , 2013, 50, 246-254. | 1.0 | 3 |
| 7191 | Modeling of two- and three-ring aromatics formation in the pyrolysis of toluene. <i>Proceedings of the Combustion Institute</i> , 2013, 34, 269-277. | 2.4 | 90 |
| 7192 | Exploring the capabilities of TDDFT calculations to explain the induced chirality upon a binding process: A simple case, 3-carboxycoumarin. <i>Journal of Molecular Structure</i> , 2013, 1036, 341-349. | 1.8 | 11 |
| 7193 | Energetics of H-atom addition to naphthalene: A thermochemical cycle from tetralin to naphthalene. <i>Journal of Chemical Thermodynamics</i> , 2013, 61, 83-89. | 1.0 | 3 |
| 7194 | Relativistic time-dependent density functional calculations for the excited states of the cadmium dimer. <i>Chemical Physics</i> , 2013, 415, 112-118. | 0.9 | 2 |
| 7195 | Fluorinated bis(phenoxy-imine)titanium complexes with methylaluminoxane for the synthesis of ultra high molecular weight polyethylene. <i>Polymer</i> , 2013, 54, 3217-3222. | 1.8 | 6 |
| 7196 | Zone centre phonon frequencies for lithium manganese oxides $\text{Li}_x\text{Mn}_2\text{O}_4$ ($x=1, 0.5$ and 0.015). <i>Computational Materials Science</i> , 2013, 77, 384-386. | 1.4 | 2 |
| 7197 | Computational study on the molecular structures and photoelectron spectra of bimetallic oxide clusters (M=V, Nb, Ta). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 109, 125-132. | 2.0 | 8 |
| 7198 | A theoretical study of factors affecting corrosion in supercritical water reaction vessels. <i>Journal of Supercritical Fluids</i> , 2013, 79, 261-267. | 1.6 | 10 |
| 7199 | Radical cations from diarylamino-substituted fluorenones. <i>Tetrahedron Letters</i> , 2013, 54, 35-39. | 0.7 | 5 |
| 7200 | Theoretical study of hydrogen adsorption on Co clusters. <i>Computational and Theoretical Chemistry</i> , 2013, 1021, 183-190. | 1.1 | 13 |
| 7201 | Benchmark calculations of density functionals for organothiol adsorption on gold surfaces. <i>Computational and Theoretical Chemistry</i> , 2013, 1009, 60-69. | 1.1 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7202 | Electronic absorption, vibrational spectra, nonlinear optical properties, NBO analysis and thermodynamic properties of N-(4-nitro-2-phenoxyphenyl) methanesulfonamide molecule by ab initio HF and density functional methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 108, 186-196. | 2.0 | 51 |
| 7203 | Domino synthesis of protochromic α -ON β -OFF α -ON β -luminescent 2-styryl quinolines. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 2597. | 1.5 | 21 |
| 7204 | Electron-Rich Trialkyl-Type Dihydro-KITPHOS Monophosphines: Efficient Ligands for Palladium-Catalyzed Suzuki-Miyaura Cross-Coupling. Comparison with Their Biaryl-Like KITPHOS Monophosphine Counterparts. <i>Organometallics</i> , 2013, 32, 1773-1788. | 1.1 | 26 |
| 7205 | A polarizable embedding DFT study of one-photon absorption in fluorescent proteins. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4735. | 1.3 | 44 |
| 7206 | Asararenes—A Family of Large Aromatic Macrocycles. <i>Chemistry - A European Journal</i> , 2013, 19, 3860-3868. | 1.7 | 62 |
| 7207 | Benchmarking Time-Dependent Density Functional Theory for Excited State Geometries of Organic Molecules in Gas-Phase and in Solution. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2209-2220. | 2.3 | 123 |
| 7208 | Copper(I)/silver(I)-phosphine-N-((2-pyridyl)methylidene)-6-coumarin complexes: Syntheses, structures, redox interconversion, photophysical properties and DFT computation. <i>Polyhedron</i> , 2013, 51, 27-40. | 1.0 | 15 |
| 7209 | Assessing the Accuracy of Density Functional and Semiempirical Wave Function Methods for Water Nanoparticles: Comparing Binding and Relative Energies of (H ₂ O) ₁₆ and (H ₂ O) ₁₇ to CCSD(T) Results. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 995-1006. | 2.3 | 51 |
| 7210 | Copper-Catalyzed Direct Ortho-Alkylation of N-Iminopyridinium Ylides with N-Tosylhydrazones. <i>Journal of Organic Chemistry</i> , 2013, 78, 3879-3885. | 1.7 | 90 |
| 7211 | Diels-Alder and Retro-Diels-Alder Cycloadditions of (1,2,3,4,5-pentamethyl)cyclopentadiene to La@C ₂ v@C ₈₂ : Regioselectivity and Product Stability. <i>Chemistry - A European Journal</i> , 2013, 19, 4468-4479. | 1.7 | 27 |
| 7212 | Chitosan as a green inhibitor for copper corrosion in acidic medium. <i>International Journal of Biological Macromolecules</i> , 2013, 55, 142-149. | 3.6 | 218 |
| 7213 | Metal-metal interactions in deltahedral dirhoda- and diiridadicarbaboranes. <i>Inorganica Chimica Acta</i> , 2013, 397, 83-87. | 1.2 | 17 |
| 7214 | Neighboring Effect in Fragmentation Pathways of Cage Guanlylhydrazones in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2242-2252. | 1.1 | 5 |
| 7215 | Density Functional Theory Study of the Mechanisms of Iron-Catalyzed Cross-Coupling Reactions of Alkyl Grignard Reagents. <i>Journal of Physical Chemistry A</i> , 2013, 117, 756-764. | 1.1 | 23 |
| 7216 | Aminoxyl (Nitroxyl) Radicals in the Early Decomposition of the Nitramine RDX. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2233-2241. | 1.1 | 25 |
| 7217 | Reactivity Models of Hydrogen Activation by Frustrated Lewis Pairs: Synergistic Electron Transfers or Polarization by Electric Field?. <i>Journal of the American Chemical Society</i> , 2013, 135, 4425-4437. | 6.6 | 193 |
| 7218 | Theoretical study on the mechanism and kinetics of addition of hydroxyl radicals to fluorobenzene. <i>Journal of Computational Chemistry</i> , 2013, 34, 646-655. | 1.5 | 17 |
| 7219 | Evaluation of Absolute Hardness: A New Approach. <i>Journal of Physical Chemistry A</i> , 2013, 117, 939-946. | 1.1 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7220 | Facile Synthesis of 2-Substituted Benzo[b]thiophen-3-ols in Water. <i>Synthetic Communications</i> , 2013, 43, 1337-1344. | 1.1 | 6 |
| 7221 | Synthesis, Magnetic Properties, and Phosphoesterase Activity of Dinuclear Cobalt(II) Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 2029-2043. | 1.9 | 62 |
| 7222 | Natural bond orbital, nuclear magnetic resonance analysis and hybrid-density functional theory study of π -aromaticity in Al ₂ F ₆ , Al ₂ Cl ₆ , Al ₂ Br ₆ and Al ₂ I ₆ . <i>Journal of Molecular Modeling</i> , 2013, 19, 2549-2557. | 0.8 | 7 |
| 7223 | Theoretical study on the solvent influence on 1,2,3-triazole tautomeric equilibrium. A comparison of incremental microsolvation and continuum solvation model approaches. <i>Tetrahedron</i> , 2013, 69, 3197-3205. | 1.0 | 7 |
| 7224 | Indeno[2,1- <i>c</i>]fluorene: A New Electron-Accepting Scaffold for Organic Electronics. <i>Organic Letters</i> , 2013, 15, 1362-1365. | 2.4 | 126 |
| 7225 | Torsional barriers of substituted biphenyls calculated using density functional theory: a benchmarking study. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 2859. | 1.5 | 51 |
| 7226 | <i>Ab Initio</i> Periodic Simulation of the Spectroscopic and Optical Properties of Novel Porous Graphene Phases. <i>Journal of Physical Chemistry C</i> , 2013, 117, 2222-2229. | 1.5 | 33 |
| 7227 | CO Adsorption on a Mixed-Valence Ruthenium Metal-Organic Framework Studied by UHV-FTIR Spectroscopy and DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 5658-5666. | 1.5 | 48 |
| 7228 | Revisiting the optical signatures of BODIPY with <i>ab initio</i> tools. <i>Chemical Science</i> , 2013, 4, 1950. | 3.7 | 140 |
| 7229 | Control of the Helical Chirality of Enantiopure Sulfinyl (<i>Z</i>)-Azobenzene-Based Photoswitches. <i>Chemistry - A European Journal</i> , 2013, 19, 3397-3406. | 1.7 | 12 |
| 7230 | Copper(II) Complexes of 3,4,5-Trisubstituted Pyrazolates: <i>In Situ</i> Formation of Pyrazole Rings from Different Carbon Centers. <i>Chemistry - an Asian Journal</i> , 2013, 8, 623-629. | 1.7 | 4 |
| 7231 | Influence of the chloro substituent on the mesomorphism of unsymmetrical achiral four-ring bent-core compounds: 2D polarization modulated banana phases. <i>Journal of Materials Chemistry C</i> , 2013, 1, 663-670. | 2.7 | 31 |
| 7232 | Unraveling the Pathway of Gold(I)-Catalyzed Olefin Hydrogenation: An Ionic Mechanism. <i>Journal of the American Chemical Society</i> , 2013, 135, 1295-1305. | 6.6 | 53 |
| 7233 | DFT Studies of Trans and Cis Influences in the Homolysis of the Co-C Bond in Models of the Alkylcobalamins. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3057-3068. | 1.1 | 19 |
| 7234 | Modeling Transition Metal Reactions with Range-Separated Functionals. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2286-2299. | 2.3 | 21 |
| 7235 | Electronic structure and optical spectra of semiconducting carbon nanotubes functionalized by diazonium salts. <i>Chemical Physics</i> , 2013, 413, 89-101. | 0.9 | 42 |
| 7236 | A new family of four-ring bent-core nematic liquid crystals with a highly polar end-group. <i>Liquid Crystals</i> , 2013, 40, 120-129. | 0.9 | 17 |
| 7237 | n-Diamond: Dynamical stability of proposed structures. <i>Diamond and Related Materials</i> , 2013, 34, 60-64. | 1.8 | 12 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7238 | Atropisomers of Arylmaleimides: Stereodynamics and Absolute Configuration. <i>Journal of Organic Chemistry</i> , 2013, 78, 3709-3719. | 1.7 | 32 |
| 7239 | Synthesis and Structural Characterization of Heteroboroxines with MB ₂ O ₃ Core (M = Sb, Bi, Sn). <i>Inorganic Chemistry</i> , 2013, 52, 1424-1431. | 1.9 | 22 |
| 7240 | Assessment of density functional methods for thermochemistry of chromium oxo compounds and their application in a study of chromia-silica system. <i>Chemical Physics Letters</i> , 2013, 561-562, 87-91. | 1.2 | 15 |
| 7241 | Magnetic interactions in oxide-bridged dichromium(III) complexes. Computational determination of the importance of non-bridging ligands. <i>Inorganica Chimica Acta</i> , 2013, 396, 72-77. | 1.2 | 10 |
| 7242 | Molecular structure and spectroscopy of divalent first row transition metals, Mn-Zn, with salicylaldiminate ligands. <i>Polyhedron</i> , 2013, 54, 300-308. | 1.0 | 7 |
| 7243 | Complex consequences: Substituent effects on metal-arylmethyl cation interactions. <i>Journal of Organometallic Chemistry</i> , 2013, 748, 68-74. | 0.8 | 6 |
| 7245 | Performance of Non-Local and Atom-Pairwise Dispersion Corrections to DFT for Structural Parameters of Molecules with Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 308-315. | 2.3 | 91 |
| 7246 | Exciton Coupling Mechanisms Analyzed with Subsystem TDDFT: Direct vs Pseudo Exchange Effects. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3480-3487. | 1.2 | 17 |
| 7247 | Monomeric Rhodium(II) Complexes Supported by a Diarylamido/Bis(phosphine) PNP Pincer Ligand and Their Reactivity Toward Dihydrogen. <i>Organometallics</i> , 2013, 32, 2050-2058. | 1.1 | 32 |
| 7248 | Theoretical studies on the spectroscopic properties of a series of palladium (II) complexes with 1-allyl-3-(2-pyridyl)thiourea. <i>Synthetic Metals</i> , 2013, 167, 51-63. | 2.1 | 6 |
| 7249 | On the performance of long-range corrected density functional theory and reduced-size polarized LPol basis sets in computations of electric dipole (hyper)polarizabilities of conjugated molecules. <i>Journal of Computational Chemistry</i> , 2013, 34, 819-826. | 1.5 | 28 |
| 7250 | Theoretical studies on the transport mechanism of 5-fluorouracil through cyclic peptide based nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 1260-1270. | 1.3 | 32 |
| 7251 | On the triplet instability in TDDFT. <i>Molecular Physics</i> , 2013, 111, 1271-1274. | 0.8 | 50 |
| 7252 | Nonamethylcyclopentyl Cation Rearrangement Mysteries Solved. <i>Organic Letters</i> , 2013, 15, 1725-1727. | 2.4 | 4 |
| 7253 | Cholesterol-based dimeric liquid crystals: synthesis, mesomorphic behaviour of frustrated phases and DFT study. <i>Liquid Crystals</i> , 2013, 40, 468-481. | 0.9 | 45 |
| 7254 | Electron-Deficient ¹ -Indenyl, ³ -allylpalladium(II) Complexes Stabilized by Fluxional Non-covalent Interactions. <i>Journal of the American Chemical Society</i> , 2013, 135, 1715-1718. | 6.6 | 23 |
| 7255 | Intramolecular Oxyallyl-Carbonyl (3 + 2) Cycloadditions. <i>Journal of the American Chemical Society</i> , 2013, 135, 5242-5245. | 6.6 | 42 |
| 7256 | On the Influence of Water on the Electronic Structure of Firefly Oxyluciferin Anions from Absorption Spectroscopy of Bare and Monohydrated Ions in Vacuo. <i>Journal of the American Chemical Society</i> , 2013, 135, 6485-6493. | 6.6 | 55 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7257 | Investigating the Structure of Aggregates of an Amphiphilic Cyanine Dye with Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5857-5867. | 1.2 | 22 |
| 7258 | Use of <i>ab initio</i> methods for the interpretation of the experimental IR reflectance spectra of crystalline compounds. <i>Journal of Computational Chemistry</i> , 2013, 34, 1476-1485. | 1.5 | 12 |
| 7259 | Oxygen-Assisted Hydroxymatairesinol Dehydrogenation: A Selective Secondary Alcohol Oxidation over a Gold Catalyst. <i>Chemistry - A European Journal</i> , 2013, 19, 4577-4585. | 1.7 | 13 |
| 7260 | Gold(I)-Catalyzed Formation of Bicyclo[4.2.0]oct-1-enes. <i>Journal of Organic Chemistry</i> , 2013, 78, 5685-5690. | 1.7 | 22 |
| 7261 | EH ₃ (E=N, P, As) and H ₂ Activation with N-Heterocyclic Silylene and Germylene Homologues. <i>Chemistry - A European Journal</i> , 2013, 19, 7835-7846. | 1.7 | 29 |
| 7262 | Olefin Hydrosilylation Catalyzed by a Bis-N-Heterocyclic Carbene Rhodium Complex. A Density Functional Theory Study. <i>Organometallics</i> , 2013, 32, 2363-2372. | 1.1 | 18 |
| 7263 | State-Specific Embedding Potentials for Excitation-Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2355-2367. | 2.3 | 70 |
| 7264 | Hierarchy of Relative Bond Dissociation Enthalpies and Their Use to Efficiently Compute Accurate Absolute Bond Dissociation Enthalpies for C-H, C-C, and C-F Bonds. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3666-3675. | 1.1 | 32 |
| 7265 | Extended Hückel Theory for Carbon Nanotubes: Band Structure and Transport Properties. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3650-3654. | 1.1 | 13 |
| 7266 | A quantum chemical view of enthalpy-entropy compensation. <i>MedChemComm</i> , 2013, 4, 1025. | 3.5 | 15 |
| 7267 | Multiconfigurational Self-Consistent Field Calculations of the Magnetically Induced Current Density Using Gauge-Including Atomic Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2189-2198. | 2.3 | 34 |
| 7268 | Subtle <i>supramolecular buttressing effects</i> in Cucurbit[7]uril/guest assemblies. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 3116. | 1.5 | 11 |
| 7269 | Mechanistic Insights into Copper-Catalyzed Sonogashira-Hagihara-Type Cross-Coupling Reactions: Sub-Mol% Catalyst Loadings and Ligand Effects. <i>Chemistry - A European Journal</i> , 2013, 19, 8144-8152. | 1.7 | 72 |
| 7270 | An improved B3LYP method in the calculation of organic thermochemistry and reactivity. <i>Computational and Theoretical Chemistry</i> , 2013, 1015, 64-71. | 1.1 | 56 |
| 7271 | Synthesis, characterization and catalytic activity of copper(ii) complexes containing a redox-active benzoxazole iminosemiquinone ligand. <i>Dalton Transactions</i> , 2013, 42, 6829. | 1.6 | 53 |
| 7272 | Structural, vibrational, electronic and NMR spectral analysis of benzyl phenyl carbonate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 110, 169-178. | 2.0 | 9 |
| 7273 | What Can We Learn about Dispersion from the Conformer Surface of <i>n</i> -Pentane?. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3118-3132. | 1.1 | 60 |
| 7274 | Nickel(II) complexes with bridged polyamines. <i>Polyhedron</i> , 2013, 56, 1-8. | 1.0 | 5 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7275 | Advanced chemical recycling of poly(ethylene terephthalate) through organocatalytic aminolysis. <i>Polymer Chemistry</i> , 2013, 4, 1610-1616. | 1.9 | 136 |
| 7276 | Computational analysis of substituent effects and Hammett constants for the ionization of gas phase acids. <i>Computational and Theoretical Chemistry</i> , 2013, 1008, 46-51. | 1.1 | 6 |
| 7277 | Benzenation of graphene upon addition of monovalent chemical species. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6842. | 1.3 | 21 |
| 7278 | Direct determination of exciton couplings from subsystem time-dependent density-functional theory within the Tamm-Dancoff approximation. <i>Journal of Chemical Physics</i> , 2013, 138, 034104. | 1.2 | 41 |
| 7279 | A RASSCF study of free base, magnesium and zinc porphyrins: accuracy versus efficiency. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 2197. | 1.3 | 17 |
| 7280 | Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2749-2760. | 2.3 | 243 |
| 7281 | Electrochemical and Catalytic Studies of a Manganese(III) Complex with a Tetradentate Schiff Base Ligand Encapsulated in NaY Zeolite. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 2768-2776. | 1.0 | 10 |
| 7282 | Assessing the viability of biosynthetic pathways for calophylline A formation—are pericyclic reactions involved?. <i>Tetrahedron Letters</i> , 2013, 54, 2952-2955. | 0.7 | 6 |
| 7283 | Conformational Preference of Fused Carbohydrate-Templated Proline Analogues—A Computational Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 199-205. | 1.2 | 3 |
| 7284 | Effect of the chemical modifications of thiophene-based N3 dyes on the performance of dye-sensitized solar cells: A density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2013, 1015, 8-14. | 1.1 | 21 |
| 7285 | Accurate Study of the Two Lowest Singlet States of HN_3 : Stationary Structures and Energetics at the MRCI Complete Basis Set Limit. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4044-4050. | 1.1 | 7 |
| 7286 | Quantum chemical approach toward the electronic, photophysical and charge transfer properties of the materials used in organic field-effect transistors. <i>Materials Chemistry and Physics</i> , 2013, 138, 468-478. | 2.0 | 26 |
| 7287 | On structure and bonding of lanthanoid trifluorides LnF_3 (Ln = La to Lu). <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 7839. | 1.3 | 25 |
| 7288 | Chalcogen—Nitrogen Secondary Bonding Interactions in the Gas Phase—Spectrometric Detection of Ionized Benzo[2,1,3]telluradiazole Dimers. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 2751-2756. | 1.0 | 25 |
| 7289 | Propan-2-ol dehydration on H-ZSM-5 and H-Y zeolite: a DFT study. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2013, 108, 565-582. | 0.8 | 17 |
| 7290 | Unraveling the Enigmatic Mechanism of $\text{Asp}^{\text{sc}}\text{Asp}^{\text{sc}}$ -Asparaginase II with QM/QM Calculations. <i>Journal of the American Chemical Society</i> , 2013, 135, 7146-7158. | 6.6 | 57 |
| 7291 | X-ray Crystallographic and First-Principles Theoretical Studies of $\text{K}_2[\text{TcOCl}_5]$ and UV/Vis Investigation of the $[\text{TcOCl}_5]^{2-}$ and $[\text{TcOCl}_4]^{2-}$ Ions. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 1097-1104. | 1.0 | 3 |
| 7292 | Research on the chelation between luteolin and Cr(III) ion through infrared spectroscopy, UV-vis spectrum and theoretical calculations. <i>Journal of Molecular Structure</i> , 2013, 1034, 386-391. | 1.8 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7293 | Quantum Mechanics/Molecular Mechanics Modeling of Regioselectivity of Drug Metabolism in Cytochrome P450 2C9. <i>Journal of the American Chemical Society</i> , 2013, 135, 8001-8015. | 6.6 | 110 |
| 7294 | TD-DFT study on the charge-transfer excitations of anions possessing double or triple bonds. <i>Computational and Theoretical Chemistry</i> , 2013, 1014, 49-55. | 1.1 | 4 |
| 7295 | Two halosesquiterpenes from <i>Laurencia composita</i> . <i>RSC Advances</i> , 2013, 3, 1953-1956. | 1.7 | 14 |
| 7296 | Comparative evaluation of a Pictet-Spengler protocol in microwave-assisted conversions of tryptamine with aryl- and carboxyaryl aldehydes: role of ring strain in cyclocondensation of the primarily formed carboxyaryl-substituted β^2 -carbolines. <i>Monatshefte für Chemie</i> , 2013, 144, 1381-1387. | 0.9 | 10 |
| 7297 | Structural and magnetic characterizations of the first manganese(III) Schiff base complexes involving hexathiocyanidoplatinate(IV) bridges. <i>CrystEngComm</i> , 2013, 15, 5351. | 1.3 | 9 |
| 7298 | The Melatonin Conformer Space: Benchmark and Assessment of Wave Function and DFT Methods for a Paradigmatic Biological and Pharmacological Molecule. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2269-2277. | 1.1 | 91 |
| 7299 | Structure and Bonding in Ionized Water Clusters. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5385-5391. | 1.1 | 41 |
| 7300 | Insight into One-Electron Oxidation of the $\{Fe(NO)_2\}^9$ Dinitrosyl Iron Complex (DNIC): Aminyl Radical Stabilized by $[Fe(NO)_2]$ Motif. <i>Inorganic Chemistry</i> , 2013, 52, 1631-1639. | 1.9 | 36 |
| 7301 | Methanol clusters (CH ₃ OH) _n : Putative global minimum-energy structures from model potentials and dispersion-corrected density functional theory. <i>Journal of Chemical Physics</i> , 2013, 138, 224303. | 1.2 | 42 |
| 7302 | Mechanistic investigation of Cu(I)-mediated three-component domino reaction of asymmetrical alkynes with carbon dioxide: Theoretical rationale for the regioselectivity. <i>Journal of Organometallic Chemistry</i> , 2013, 748, 84-88. | 0.8 | 9 |
| 7303 | Efficient Methods for the Quantum Chemical Treatment of Protein Structures: The Effects of London-Dispersion and Basis-Set Incompleteness on Peptide and Water-Cluster Geometries. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3240-3251. | 2.3 | 75 |
| 7304 | Probing the Smallest Molecular Model of MoS ₂ Catalyst: S ₂ Units in the MoS _n ($n = 1-5$) Clusters. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5632-5641. | 1.1 | 21 |
| 7305 | Detailed EPR Study of Spin Crossover Dendrimeric Iron(III) Complex. <i>Journal of Physical Chemistry B</i> , 2013, 117, 7833-7842. | 1.2 | 35 |
| 7306 | <i>N</i> -Alkylation of Chiral Tropane- and Homotropane-Derived Enamines. <i>Journal of Organic Chemistry</i> , 2013, 78, 1508-1518. | 1.7 | 12 |
| 7307 | Effect of Imide Functionalization on the Electronic, Optical, and Charge Transport Properties of Coronene: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 825-836. | 1.5 | 52 |
| 7308 | Assessment of density functional methods with correct asymptotic behavior. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 8352. | 1.3 | 49 |
| 7309 | Computational Investigations on Base-Catalyzed Diaryl Ether Formation. <i>Journal of Organic Chemistry</i> , 2013, 78, 5436-5443. | 1.7 | 20 |
| 7310 | Highly-efficient charge separation and polaron delocalization in polymer-fullerene bulk-heterojunctions: a comparative multi-frequency EPR and DFT study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9562. | 1.3 | 135 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7311 | Conformational analysis of azepane, oxepane, silepane, phosphepane, thiepane and the azepanium cation by high level quantum mechanics. <i>Structural Chemistry</i> , 2013, 24, 751-762. | 1.0 | 5 |
| 7312 | Simulating Ru L ₃ -Edge X-ray Absorption Spectroscopy with Time-Dependent Density Functional Theory: Model Complexes and Electron Localization in Mixed-Valence Metal Dimers. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4444-4454. | 1.1 | 59 |
| 7313 | Analytic derivatives for the XYG3 type of doubly hybrid density functionals: Theory, implementation, and assessment. <i>Journal of Computational Chemistry</i> , 2013, 34, 1759-1774. | 1.5 | 26 |
| 7314 | Asymmetric Synthesis of (1,5)Naphthalenophanes by Dehydro α -Diels β -Alder Reaction. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 2123-2129. | 1.2 | 13 |
| 7315 | Substituent Effects in the Absorption Spectra of Phenol Radical Species: Origin of the Redshift Caused by 3,5 α -Dimethoxyl Substitution. <i>Photochemistry and Photobiology</i> , 2013, 89, 536-544. | 1.3 | 2 |
| 7316 | Organic Single Molecular Structures for Light Induced Spin-Pump Devices. <i>ACS Nano</i> , 2013, 7, 1064-1071. | 7.3 | 26 |
| 7317 | <i>Cis</i> Carotenoids: Colorful Molecules and Free Radical Quenchers. <i>Journal of Physical Chemistry B</i> , 2013, 117, 4050-4061. | 1.2 | 27 |
| 7318 | Crystal Packing and Magnetism in Phenolic Nitronyl Nitroxides: 2-(3 α ,5 α -Dimethoxy-4 α -hydroxyphenyl)-4,4,5,5-tetramethyl-4,5-dihydro-1 <i>H</i> -imidazole-1-oxyl. <i>Crystal Growth and Design</i> , 2013, 13, 893-900. | 1.4 | 6 |
| 7319 | Molecular, crystal, and electronic structure of the cobalt(II) complex with 10-(2-benzothiazolylazo)-9-phenanthrol. <i>Crystallography Reports</i> , 2013, 58, 427-436. | 0.1 | 4 |
| 7320 | Interaction Modes and Absolute Affinities of α -Amino Acids for Mn ²⁺ : A Comprehensive Picture. <i>ChemPhysChem</i> , 2013, 14, 1733-1745. | 1.0 | 9 |
| 7321 | Effect of Distal Interactions on O ₂ Binding to Heme. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3755-3770. | 1.2 | 39 |
| 7322 | Understanding the Density Functional Dependence of DFT-Calculated Electronic Couplings in Organic Semiconductors. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 919-924. | 2.1 | 79 |
| 7323 | Energies and Spin States of FeS ₀ ⁺ , FeS ₂ ⁺ , FeS ₂ S ₂ ⁺ , FeS ₃ S ₄ ⁺ , and FeS ₄ S ₄ ⁺ Clusters. <i>ChemPhysChem</i> , 2013, 14, 1182-1189. | 1.0 | 8 |
| 7324 | Blending Through-Space and Through-Bond π - π -Coupling in [2,2 α]-Paracyclophane-oligophenylenevinylene Molecular Wires. <i>Journal of the American Chemical Society</i> , 2013, 135, 10372-10381. | 6.6 | 66 |
| 7325 | Assessment of range-separated time-dependent density-functional theory for calculating <i>C</i> ₆ dispersion coefficients. <i>Journal of Chemical Physics</i> , 2013, 138, 194106. | 1.2 | 20 |
| 7326 | Ultrafast Excited-State Dynamics of <i>ortho</i> -Terphenyl and 1,2-Diphenylcyclohexene: The Role of α Ethylenic Twisting β in the Nonadiabatic Photocyclization of Stilbene Analogs. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1895-1900. | 2.1 | 13 |
| 7327 | Bisguanidines with Biphenyl, Binaphthyl, and Bipyridyl Cores: Proton α Sponge Properties and Coordination Chemistry. <i>Chemistry - A European Journal</i> , 2013, 19, 8958-8977. | 1.7 | 23 |
| 7328 | Possibility of Having HF-Doped Hydrogen Hydrates. <i>Journal of Physical Chemistry C</i> , 2013, 117, 11625-11634. | 1.5 | 14 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7329 | Noninteracting, Vicinal Frustrated P/B-Lewis Pair at the Norbornane Framework: Synthesis, Characterization, and Reactions. <i>Journal of the American Chemical Society</i> , 2013, 135, 8882-8895. | 6.6 | 89 |
| 7330 | From N-benzoylpyridinium imides to pyrazolo[1,5-a]pyridines: a mechanistic discussion on a stoichiometric Cu protocol. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 3894. | 1.5 | 27 |
| 7331 | Improved Predictor–Corrector Integrators For Evaluating Reaction Path Curvature. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1481-1488. | 2.3 | 27 |
| 7332 | Studies on structures and electron affinities of the simplest alkyl dithio radicals and their anions with gaussian-3 theory and density functional theory. <i>Journal of Molecular Modeling</i> , 2013, 19, 2443-2449. | 0.8 | 4 |
| 7333 | Intermolecular Interactions in Crystalline Theobromine as Reflected in Electron Deformation Density and ¹³ C NMR Chemical Shift Tensors. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2629-2638. | 2.3 | 22 |
| 7334 | On the gas-phase dimerization of negatively charged closo-dodecaborates: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10358. | 1.3 | 10 |
| 7335 | Oxidative addition transition states of Pd(0) complexes in polar solvent—a DFT study involving implicit and explicit solvation. <i>Tetrahedron</i> , 2013, 69, 5715-5718. | 1.0 | 32 |
| 7336 | Understanding the Equilibria of Thio Compounds Adsorbed on Gold by Surface-Enhanced Raman Scattering and Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 6275-6283. | 1.5 | 17 |
| 7337 | Switching of Reverse Charge Transfers for a Rational Design of an OFF–ON Phosphorescent Chemodosimeter of Cyanide Anions. <i>Inorganic Chemistry</i> , 2013, 52, 4890-4897. | 1.9 | 58 |
| 7338 | Synthesis and characterization of new electron acceptor perylene diimide molecules for photovoltaic applications. <i>Dyes and Pigments</i> , 2013, 99, 329-338. | 2.0 | 56 |
| 7339 | Caryolene-forming carbocation rearrangements. <i>Beilstein Journal of Organic Chemistry</i> , 2013, 9, 323-331. | 1.3 | 23 |
| 7340 | Fullerenes toxicity and electronic properties. <i>Environmental Chemistry Letters</i> , 2013, 11, 105-118. | 8.3 | 44 |
| 7341 | Insights into the Catalytic Mechanism of Coral Allene Oxide Synthase: A Dispersion Corrected Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 6701-6710. | 1.2 | 21 |
| 7342 | Theoretical Studies on Nickel-Catalyzed Cycloaddition of 3-Azetidinone with Alkynes. <i>Organometallics</i> , 2013, 32, 3003-3011. | 1.1 | 36 |
| 7343 | On the Metric of Charge Transfer Molecular Excitations: A Simple Chemical Descriptor. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3118-3126. | 2.3 | 335 |
| 7344 | Periodic Trends in 3d Metal Mediated CO ₂ Activation. <i>ACS Symposium Series</i> , 2013, , 67-88. | 0.5 | 3 |
| 7345 | Chirality Control for in Situ Preparation of Gold Nanoparticle Superstructures Directed by a Coordinatable Organogelator. <i>Journal of the American Chemical Society</i> , 2013, 135, 9174-9180. | 6.6 | 68 |
| 7346 | Removal of Mercury from the Environment: A Quantum-Chemical Study with the Normalized Elimination of the Small Component Method. <i>Inorganic Chemistry</i> , 2013, 52, 2497-2504. | 1.9 | 28 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7347 | Conjugated donor-acceptor (D-A) copolymers in inverted organic solar cells – a combined experimental and modelling study. <i>Journal of Materials Chemistry A</i> , 2013, 1, 7451. | 5.2 | 13 |
| 7348 | Bis(carbazolyl) derivatives of pyrene and tetrahydropyrene: synthesis, structures, optical properties, electrochemistry, and electroluminescence. <i>Journal of Materials Chemistry C</i> , 2013, 1, 1638. | 2.7 | 77 |
| 7349 | Hypoelectronic diruthenaboranes and diosmaboranes having eight to twelve vertices: capped isocloso and bicapped closo structures. <i>New Journal of Chemistry</i> , 2013, 37, 2528. | 1.4 | 3 |
| 7350 | Selecting DFT methods for use in optimizations of enzyme active sites: applications to ONIOM treatments of DNA glycosylases. <i>Canadian Journal of Chemistry</i> , 2013, 91, 559-572. | 0.6 | 16 |
| 7351 | Robustness of Frequency, Transition Dipole, and Coupling Maps for Water Vibrational Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3109-3117. | 2.3 | 86 |
| 7352 | Nuclear spin-spin coupling anisotropy in the van der Waals-bonded ¹²⁹ Xe dimer. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 11427. | 1.3 | 6 |
| 7353 | Comparison of hypoelectronic deltahedral ditechneboranes having eight to twelve vertices with their rhenium analogues: Examples of polyhedral surface metal-metal multiple bonds. <i>Polyhedron</i> , 2013, 60, 151-157. | 1.0 | 8 |
| 7354 | First Principles Studies of the Vibrationally Resolved Magnetic Circular Dichroism Spectra of Biphenylene. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1557-1567. | 2.3 | 19 |
| 7355 | How the Quantum Efficiency of a Highly Emissive Binuclear Copper Complex Is Enhanced by Changing the Processing Solvent. <i>Langmuir</i> , 2013, 29, 3034-3044. | 1.6 | 54 |
| 7356 | A Caveat on SCC-DFTB and Noncovalent Interactions Involving Sulfur Atoms. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3020-3025. | 2.3 | 13 |
| 7357 | Boranil and Related NBO Dyes: Insights From Theory. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3127-3135. | 2.3 | 74 |
| 7358 | Small Optical Gap Molecules and Polymers: Using Theory to Design More Efficient Materials for Organic Photovoltaics. <i>Topics in Current Chemistry</i> , 2013, 352, 1-38. | 4.0 | 14 |
| 7359 | Formation of (E)-[FcC(PS ₂ (OR) ₂)CH(PS ₂ (OR) ₂)] (R=Me, Et, Pr) in photolytic reactions of ferrocenylacetylene and [(RO) ₂ PS ₂ H] in hexane/alcohols: Experimental and DFT study. <i>Journal of Organometallic Chemistry</i> , 2013, 748, 46-50. | 0.8 | 2 |
| 7360 | Leucotrichoic acid, a novel sesquiterpene from <i>Sinningia leucotricha</i> (Gesneriaceae). <i>Tetrahedron Letters</i> , 2013, 54, 4735-4737. | 0.7 | 9 |
| 7361 | RELATIONSHIPS BETWEEN DIFFERENT-ORDER POLARIZABILITIES AND GROUND STATE DIPOLE MOMENT. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1250099. | 1.8 | 20 |
| 7362 | Influence of Crystal Packing on an Organometallic Ruthenium(IV) Complex Structure: The Right Distance for the Right Reason. <i>Organometallics</i> , 2013, 32, 3784-3787. | 1.1 | 27 |
| 7363 | Orbital Analysis and Excited-State Calculations in an Energy-Based Fragmentation Method. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3350-3363. | 2.3 | 9 |
| 7364 | Prediction of Redox Potentials of Adrenaline and Its Supramolecular Complex with Glycine: Theoretical and Experimental Studies. <i>Journal of Physical Chemistry B</i> , 2013, 117, 2081-2087. | 1.2 | 10 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 7365 | On the oxidation state of iron in iron-mediated C–C couplings. <i>Journal of Organometallic Chemistry</i> , 2013, 748, 51-55. | 0.8 | 50 |
| 7366 | Aromatic ring size effects on the photophysics and photochemistry of styrylbenzothiazole. <i>Photochemical and Photobiological Sciences</i> , 2013, 12, 1220-1231. | 1.6 | 14 |
| 7367 | Oxygen Defects and Surface Chemistry of Ceria: Quantum Chemical Studies Compared to Experiment. <i>Chemical Reviews</i> , 2013, 113, 3949-3985. | 23.0 | 849 |
| 7368 | Mechanistic Studies on Water–Exchange Reactions in $[Zn(H_2O)_4L]^{2+}$ for $L = sp^2, sp^3$ Oxygen–Donor Ligands: A DFT Approach. <i>European Journal of Inorganic Chemistry</i> , 2013, 2059-2069. | 1.0 | 4 |
| 7369 | Substrate-Assisted and Nucleophilically Assisted Catalysis in Bovine β -1,3-Galactosyltransferase. Mechanistic Implications for Retaining Glycosyltransferases. <i>Journal of the American Chemical Society</i> , 2013, 135, 7053-7063. | 6.6 | 42 |
| 7370 | Structure change, layer sliding, and metallization in high-pressure MoS ₂ . <i>Physical Review B</i> , 2013, 87, . | 1.1 | 116 |
| 7371 | Aromatic Claisen Rearrangements of <i>o</i> -Prenylated Tyrosine and Model Prenyl Aryl Ethers: Computational Study of the Role of Water on Acceleration of Claisen Rearrangements. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 2823-2831. | 1.2 | 18 |
| 7372 | The spectroscopic (FTIR, FT-Raman and UV–Vis spectra), DFT and normal coordinate computations of <i>m</i> -nitromethylbenzoate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 112, 52-61. | 2.0 | 7 |
| 7373 | Ground state of a spin-crossover molecule calculated by diffusion Monte Carlo. <i>Physical Review B</i> , 2013, 87, . | 1.1 | 16 |
| 7374 | (E)-5,5-Di(thiophen-2-yl)-3,3-bis[thiophen-3(2H)-ylidene]-2,2-dione from conspicuous blue impurities to quasi-metallic golden-bronze crystals. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 3871. | 1.5 | 6 |
| 7375 | Structural Diversity from the Transannular Cyclizations of Natural Germacrone and Epoxy Derivatives: A Theoretical–Experimental Study. <i>Chemistry - A European Journal</i> , 2013, 19, 6598-6612. | 1.7 | 21 |
| 7376 | Combined ¹ H NMR and DFT study of the solvent effects on the iron pentacarbonyl-catalyzed photo-assisted isomerization of allyl alcohol. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 322-326. | 0.9 | 8 |
| 7377 | Synthesis, optical properties and charge transport characteristics of a series of novel thiophene-fused phenazine derivatives. <i>Journal of Materials Chemistry C</i> , 2013, 1, 3467. | 2.7 | 29 |
| 7378 | Performance of density functional theory in computing nonresonant vibrational (hyper)polarizabilities. <i>Journal of Computational Chemistry</i> , 2013, 34, 1775-1784. | 1.5 | 46 |
| 7379 | Chemistry of Interfacial Interactions in a LDPE-Based Nanocomposite and Their Effect on the Nanoscale Hybrid Assembling. <i>Macromolecules</i> , 2013, 46, 1563-1572. | 2.2 | 15 |
| 7380 | Comparative studies on CH–F ^{δ−} hydrogen bond formation in benzene and exocyclically substituted pentafulvene derivatives. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 575-582. | 0.9 | 4 |
| 7381 | Synthesis and Conformational Dynamics of the Reported Structure of Xylopyridine A. <i>Journal of the American Chemical Society</i> , 2013, 135, 9213-9219. | 6.6 | 16 |
| 7382 | Rubrene-Based Single-Crystal Organic Semiconductors: Synthesis, Electronic Structure, and Charge-Transport Properties. <i>Chemistry of Materials</i> , 2013, 25, 2254-2263. | 3.2 | 141 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7383 | Ab initio calculations and validation of the pH-dependent structures of the His37-Trp41 quartet, the heart of acid activation and proton conductance in the M2 protein of Influenza A virus. <i>Chemical Science</i> , 2013, 4, 2776. | 3.7 | 21 |
| 7384 | Third-Order Incremental Dual-Basis Set Zero-Buffer Approach: An Accurate and Efficient Way To Obtain CCSD and CCSD(T) Energies. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2992-3003. | 2.3 | 29 |
| 7385 | Synthesis, X-ray structural, IR spectroscopic, thermal and DFT studies of nickel(II) and copper(II) complexes with 3-methylpicolinic acid. UV-Vis spectrophotometric study of complexation in the solution. <i>Polyhedron</i> , 2013, 52, 1349-1361. | 1.0 | 17 |
| 7386 | Reactions of Iron Carbenes with α,β -Unsaturated Esters by Using an Umpolung Approach: Mechanism and Applications. <i>Chemistry - A European Journal</i> , 2013, 19, 6766-6773. | 1.7 | 18 |
| 7387 | Mechanisms of the Water-Gas Shift Reaction Catalyzed by Ruthenium Pentacarbonyl: A Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2013, 52, 4786-4794. | 1.9 | 23 |
| 7388 | Solid-phase synthesis of reduced selenocysteine tetrapeptides and their oxidized analogs containing selenenylsulfide eight-membered rings. <i>Molecular Diversity</i> , 2013, 17, 537-545. | 2.1 | 7 |
| 7389 | Probing the Role of Backbone Hydrogen Bonds in Protein-Peptide Interactions by Amide-to-Ester Mutations. <i>Journal of the American Chemical Society</i> , 2013, 135, 12998-13007. | 6.6 | 45 |
| 7390 | Energetics and Structure of Simvastatin. <i>Molecular Pharmaceutics</i> , 2013, 10, 2713-2722. | 2.3 | 26 |
| 7391 | TD-DFT benchmarks: A review. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2019-2039. | 1.0 | 938 |
| 7392 | Experimental and computational study of the energetics of hydantoin and 2-thiohydantoin. <i>Journal of Chemical Thermodynamics</i> , 2013, 58, 158-165. | 1.0 | 17 |
| 7393 | Synthesis, characterization and optical properties of low nuclearity liganded silver clusters: Ag ₃₁ (SG) ₁₉ and Ag ₁₅ (SG) ₁₁ . <i>Nanoscale</i> , 2013, 5, 5637. | 2.8 | 83 |
| 7394 | Protein induced singlet-triplet quasidegeneracy in the active site of [NiFe]-hydrogenase. <i>Chemical Physics Letters</i> , 2013, 577, 138-141. | 1.2 | 22 |
| 7395 | Class III Delocalization and Exciton Coupling in a Bimetallic Bisligand Radical Complex. <i>Chemistry - A European Journal</i> , 2013, 19, 9606-9618. | 1.7 | 32 |
| 7396 | Opposing Auxiliary Conformations Produce the Same Torquoselectivity in an Oxazolidinone-Directed Nazarov Cyclization. <i>Journal of the American Chemical Society</i> , 2013, 135, 9156-9163. | 6.6 | 43 |
| 7397 | Ultrasensitive Fiber Enhanced UV Resonance Raman Sensing of Drugs. <i>Analytical Chemistry</i> , 2013, 85, 6264-6271. | 3.2 | 75 |
| 7398 | Methane CH Activation by Palladium Complexes with Chelating Bis(NHC) Ligands: A DFT Study. <i>Organometallics</i> , 2013, 32, 3469-3480. | 1.1 | 66 |
| 7399 | Theoretical structure and vibrational spectra of ciprofloxacin: Density functional theory study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 102, 134-141. | 2.0 | 5 |
| 7400 | Experimental and computational thermochemical studies of benzoxazole and two chlorobenzoxazole derivatives. <i>Journal of Chemical Thermodynamics</i> , 2013, 57, 212-219. | 1.0 | 21 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7401 | Spectroscopic and theoretical studies of some 2-substituted N-methoxy-N-methyl-amides. <i>Journal of Molecular Structure</i> , 2013, 1031, 91-103. | 1.8 | 0 |
| 7402 | Structure of dimethylphenyl betaine hydrochloride studied by X-ray diffraction, DFT calculation, NMR and FTIR spectra. <i>Journal of Molecular Structure</i> , 2013, 1031, 49-55. | 1.8 | 9 |
| 7403 | Density functional theory study on the molecular structure and vibration spectra of fenbufen. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 101, 119-126. | 2.0 | 1 |
| 7404 | Theoretical studies on structures and electronic spectra of linear free radicals C _n H (n=5-12). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 101, 283-293. | 2.0 | 2 |
| 7405 | Evaluation of Approximate Exchange-Correlation Functionals in Predicting One-Bond ³¹ P- ¹ H NMR Indirect Spin-Spin Coupling Constants. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1443-1451. | 2.3 | 13 |
| 7406 | Coordination and Bond Activation in Complexes of Regioisomeric Phenylpyridines with the Nickel(II) Chloride Cation in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1171-1180. | 1.1 | 18 |
| 7407 | Ditopic Ambiphilicity of an Anionic Dimetalloborylene Complex. <i>Journal of the American Chemical Society</i> , 2013, 135, 2313-2320. | 6.6 | 47 |
| 7408 | An electron paramagnetic resonance and density-functional theory study on the methyl isotropic hyperfine coupling constants in gamma-irradiated 2,6-di-tert-butyl-4-methylphenol. <i>Radiation Effects and Defects in Solids</i> , 2013, 168, 206-211. | 0.4 | 2 |
| 7409 | Do silicene nanoribbons have high carrier mobilities?. <i>Europhysics Letters</i> , 2013, 101, 27005. | 0.7 | 18 |
| 7410 | Isotopic Analysis of Oxidative Pollutant Degradation Pathways Exhibiting Large H Isotope Fractionation. <i>Environmental Science & Technology</i> , 2013, 47, 13459-13468. | 4.6 | 37 |
| 7411 | Theoretical ⁵⁷ Fe Mössbauer Spectroscopy for Structure Elucidation of [Fe] Hydrogenase Active Site Intermediates. <i>Inorganic Chemistry</i> , 2013, 52, 14205-14215. | 1.9 | 24 |
| 7412 | Mechanism of Proton Transport in Ionic-Liquid-Doped Perfluorosulfonic Acid Membranes. <i>Journal of Physical Chemistry B</i> , 2013, 117, 14449-14456. | 1.2 | 23 |
| 7413 | Investigation of Astatine(III) Hydrolyzed Species: Experiments and Relativistic Calculations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1983-1990. | 1.1 | 50 |
| 7414 | Molecular Construction Kit for Tuning Solubility, Stability and Luminescence Properties: Heteroleptic MePyrPHOS-Copper Iodide-Complexes and their Application in Organic Light-Emitting Diodes. <i>Chemistry of Materials</i> , 2013, 25, 3414-3426. | 3.2 | 147 |
| 7415 | New Fe(III)(cyclam) Complexes Bearing Axially Bound <i>geminal</i> -Diethynylethenes. <i>Organometallics</i> , 2013, 32, 4684-4689. | 1.1 | 24 |
| 7416 | Mechanisms of Photodesorption of Br Atoms from CsBr Surfaces. <i>Journal of Physical Chemistry C</i> , 2013, 117, 13502-13509. | 1.5 | 6 |
| 7417 | Anionic Oligomerization of Li ₂ [B ₁₂ H ₁₂] and Li[CB ₁₁ H ₁₂]: An Experimental and Computational Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 1495-1501. | 1.5 | 7 |
| 7418 | Quantum Monte Carlo Study of π -Bonded Transition Metal Organometallics: Neutral and Cationic Vanadium-Benzene and Cobalt-Benzene Half Sandwiches. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 390-400. | 2.3 | 21 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7419 | Theoretical Study of Structural, Spectroscopic and Reaction Properties of <i>trans-bis</i> (imido) Uranium(VI) Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 9143-9152. | 1.9 | 11 |
| 7420 | Equilibrium and Rate Constants, and Reaction Mechanism of the HF Dissociation in the HF(H ₂ O) ₇ Cluster by ab Initio Rare Event Simulations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 13039-13050. | 1.1 | 13 |
| 7421 | New Class of Molecular Conductance Switches Based on the [1,3]-Silyl Migration from Silanes to Silenes. <i>Journal of Physical Chemistry C</i> , 2013, 117, 10909-10918. | 1.5 | 11 |
| 7422 | Crown Graphene Nanomeshes: Highly Stable Chelation-Doped Semiconducting Materials. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2398-2403. | 2.3 | 18 |
| 7423 | Solvated Charge Transfer States of Functionalized Anthracene and Tetracyanoethylene Dimers: A Computational Study Based on a Range Separated Hybrid Functional and Charge Constrained Self-Consistent Field with Switching Gaussian Polarized Continuum Models. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1125-1131. | 2.3 | 71 |
| 7424 | Phosphorescence Color Tuning of Cyclometalated Iridium Complexes by <i>o</i> -Carborane Substitution. <i>Inorganic Chemistry</i> , 2013, 52, 160-168. | 1.9 | 118 |
| 7425 | Tautomerism of substituted salicylaldehyde and 2-diphenylphosphinebenzaldehyde 1- <i>phthalazinylhydrazones</i> : X-ray crystallography and quantum chemical modeling. <i>Journal of Structural Chemistry</i> , 2013, 54, 952-959. | 0.3 | 4 |
| 7426 | Theoretical Exploration of Photoisomerization-Switchable Second-Order Nonlinear Optical Responses of Two-Dimensional <i>b</i> - and <i>W</i> -Shaped Polyoxometalate Derivatives of Dithienylperfluorocyclopentene. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10783-10789. | 1.1 | 20 |
| 7427 | Molecular Simulations Highlight the Role of Metals in Catalysis and Inhibition of Type II Topoisomerase. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 857-862. | 2.3 | 45 |
| 7428 | Theoretical Study of Water Oxidation by the Ruthenium Blue Dimer. II. Proton Relay Chain Mechanism for the Step [bpy ₂ (HOO)Ru ^{IV} ORu ^{IV} (OH)bpy ₂] ⁴⁺ → [bpy ₂ (O ₂)Ru ^{IV} ORu ^{III} (OH ₂)bpy ₂] ⁺ . <i>Journal of Physical Chemistry B</i> , 2013, 117, 15761-15770. | 1.2 | 10 |
| 7429 | Stepwise Protonation and Electron-Transfer Reduction of a Primary Copper ^{II} Dioxygen Adduct. <i>Journal of the American Chemical Society</i> , 2013, 135, 16454-16467. | 6.6 | 74 |
| 7430 | DFT Study of Uranyl Peroxo Complexes with H ₂ O, F ⁻ , OH ⁻ , CO ₃ ²⁻ , and NO ₃ ⁻ . <i>Inorganic Chemistry</i> , 2013, 52, 5590-5602. | 1.9 | 40 |
| 7431 | Hydroxyl Ion Addition to One-Electron Oxidized Thymine: Unimolecular Interconversion of C5 to C6 OH-Adducts. <i>Journal of the American Chemical Society</i> , 2013, 135, 3121-3135. | 6.6 | 42 |
| 7432 | Understanding Selectin Counter-Receptor Binding from Electrostatic Energy Computations and Experimental Binding Studies. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16443-16454. | 1.2 | 15 |
| 7433 | Theoretical Studies of Ring-Opening Reactions of Phenylcyclobutabenzenol and Its Reactions with Alkynes Catalyzed by Rhodium Complexes. <i>Journal of Organic Chemistry</i> , 2013, 78, 11357-11365. | 1.7 | 38 |
| 7434 | Mechanistic and Computational Studies of Exocyclic Stereocontrol in the Synthesis of Bryostatin-like <i>cis</i> -2,6-Disubstituted 4-Alkylidenetetrahydropyrans by Prins Cyclization. <i>Journal of Organic Chemistry</i> , 2013, 78, 104-115. | 1.7 | 12 |
| 7435 | Role of Spin State and Ligand Charge in Coordination Patterns in Complexes of 2,6-Diacetylpyridinebis(semioxamazide) with 3d-Block Metal Ions: A Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2013, 52, 13415-13423. | 1.9 | 19 |
| 7436 | Novel Approach to Excited-State Calculations of Large Molecules Based on Divide-and-Conquer Method: Application to Photoactive Yellow Protein. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5565-5573. | 1.2 | 36 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7437 | Origin of the Conformational Modulation of the ¹³ C NMR Chemical Shift of Methoxy Groups in Aromatic Natural Compounds. <i>Journal of Physical Chemistry A</i> , 2013, 117, 661-669. | 1.1 | 19 |
| 7438 | Effect of Substituents on the Preferred Modes of One-Electron Reductive Cleavage of Nâ€‘Cl and Nâ€‘Br Bonds. <i>Journal of Physical Chemistry A</i> , 2013, 117, 460-472. | 1.1 | 22 |
| 7439 | Toward a Broadly Applicable Force Field for d ⁶ -Piano Stool Complexes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2313-2323. | 2.3 | 6 |
| 7440 | Understanding the Site Selectivity in Small-Sized Neutral and Charged Al _n (4 %) Tj ETQq1 1 0.784314 rgBT /Ove Study on Water Molecule Adsorption. <i>Journal of Physical Chemistry A</i> , 2013, 117, 8691-8702. | 1.1 | 15 |
| 7441 | In Pursuit of Homoleptic Actinide Alkyl Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 3556-3564. | 1.9 | 42 |
| 7442 | Reaching a Uniform Accuracy for Complex Molecular Systems: Long-Range-Corrected XYG3 Doubly Hybrid Density Functional. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1669-1675. | 2.1 | 63 |
| 7443 | Closed loops theory on the third-order nonlinear optical property of π - and π^2 - isomers of [M8O26]4 ⁻ : a TDDFT study. <i>Molecular Physics</i> , 2013, 111, 3081-3086. | 0.8 | 2 |
| 7444 | Energetics of Nonbonded Ortho Interactions in Alkylbenzenes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2873-2878. | 1.1 | 5 |
| 7445 | To Jump or Not To Jump? C ¹ Hydrogen Atom Transfer in Post-cleavage Radical-Cation Complexes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1189-1196. | 1.1 | 15 |
| 7446 | O ₂ Binding to Heme is Strongly Facilitated by Nearâ€‘Degeneracy of Electronic States. <i>ChemPhysChem</i> , 2013, 14, 3551-3558. | 1.0 | 31 |
| 7447 | Combining spin-adapted open-shell TD-DFT with spinâ€‘orbit coupling. <i>Molecular Physics</i> , 2013, 111, 3741-3755. | 0.8 | 85 |
| 7448 | Theoretical investigation on the mechanism and kinetics of the ring-opening polymerization of μ -caprolactone initiated by tin(II) alkoxides. <i>Journal of Molecular Modeling</i> , 2013, 19, 5377-5385. | 0.8 | 22 |
| 7449 | Modeling opto-electronic properties of a dye molecule in proximity of a semiconductor nanoparticle. <i>Journal of Chemical Physics</i> , 2013, 139, 024105. | 1.2 | 16 |
| 7450 | Experimental and Computational Investigation of the 1,3â€‘Dipolar Cycloaddition of the Ynamide <i>tert</i> -Butyl N-Ethynyl-N-phenylcarbamate with <i>C</i> -Carboxymethyl-N-phenylnitrilimine. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 8108-8114. | 1.2 | 3 |
| 7451 | Furo[2,3- <i>c</i>]pyrans from a Vinyl Sulfone Modified Methyl 2,6-Anhydro- α -D-hexopyranoside: An Experimental and Theoretical Investigation. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 8197-8207. | 1.2 | 6 |
| 7452 | New diaminomaleonitrile derivatives containing aza-crown ether: Selective, sensitive and colorimetric chemosensors for Cu(II). <i>Dyes and Pigments</i> , 2013, 98, 1-10. | 2.0 | 46 |
| 7453 | The performance of density functional approximations for the structures and relative energies of minimum energy crossing points. <i>Chemical Physics Letters</i> , 2013, 590, 227-230. | 1.2 | 3 |
| 7454 | Molecular-level computational studies of single wall carbon nanotubeâ€‘polyethylene composites. <i>Computational Materials Science</i> , 2013, 69, 443-454. | 1.4 | 45 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7455 | Theoretical investigation on the Pt($\Delta\Delta$)-catalyzed tandem migration reactions of propargylic carboxylates. <i>Computational and Theoretical Chemistry</i> , 2013, 1019, 11-17. | 1.1 | 2 |
| 7456 | The Importance of Electron Correlation on Stacking Interaction of Adenine-Thymine Base-Pair Step in B-DNA: A Quantum Monte Carlo Study. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1081-1086. | 2.3 | 27 |
| 7457 | Phase transitions in $[\text{Co}(\text{NH}_3)_6](\text{ClO}_4)_3$ investigated by neutron scattering methods. <i>Chemical Physics</i> , 2013, 412, 1-6. | 0.9 | 3 |
| 7458 | An X-ray crystallographic and density functional theory study of (3Z)-4-(5-ethylsulfonyl-2-hydroxyanilino)pent-3-en-2-one and (3Z)-4-(5-tert-butyl-2-hydroxyanilino)pent-3-en-2-one. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2013, 69, 258-262. | 0.4 | 2 |
| 7459 | Gas-Phase Formation and Fragmentation Reactions of the Organomagnesates $[\text{RMgX}_2]^+$. <i>Organometallics</i> , 2013, 32, 2319-2328. | 1.1 | 29 |
| 7460 | Investigating the Electronic Structure of the Atox1 Copper(I) Transfer Mechanism with Density Functional Theory. <i>Inorganic Chemistry</i> , 2013, 52, 10387-10393. | 1.9 | 6 |
| 7461 | The Use of the GSAM Approach for the Structural Investigation of Low-Lying Isomers of Molecular Clusters from Density-Functional-Theory-Based Potential Energy Surfaces: The Structures of Microhydrated Nucleic Acid Bases. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7236-7245. | 1.1 | 16 |
| 7462 | Theoretical study of the Diels-Alder reaction between o-benzoquinone and norbornadiene. <i>IOP Conference Series: Materials Science and Engineering</i> , 2013, 45, 012029. | 0.3 | 1 |
| 7463 | Assessment of Tuning Methods for Enforcing Approximate Energy Linearity in Range-Separated Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4414-4420. | 2.3 | 31 |
| 7464 | Structural, Electrochemical, and Spectroscopic Investigation of Acetate Bridged Dinuclear Tetrakis-Schiff Base Macrocycles of Mn and Zn. <i>Inorganic Chemistry</i> , 2013, 52, 13963-13973. | 1.9 | 19 |
| 7465 | Distributions of methyl group rotational barriers in polycrystalline organic solids. <i>Journal of Chemical Physics</i> , 2013, 139, 204501. | 1.2 | 14 |
| 7466 | Magnetic field-induced nuclear quadrupole coupling in atomic ^{131}Xe . <i>Molecular Physics</i> , 2013, 111, 1390-1400. | 0.8 | 7 |
| 7467 | Nonplanar Tertiary Amides in Rigid Chiral Tricyclic Dilactams. Peptide Group Distortions and Vibrational Optical Activity. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9626-9642. | 1.2 | 7 |
| 7468 | Benchmark Study of the Interaction Energy for an $(\text{H}_2\text{O})_{16}$ Cluster: Quantum Monte Carlo and Complete Basis Set Limit MP2 Results. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7606-7611. | 1.1 | 20 |
| 7469 | Co-complexation Syntheses, Structural Characterization, and DFT Studies of a Novel Series of Polymeric Alkali-Metal Tetraorganogallates. <i>Organometallics</i> , 2013, 32, 480-489. | 1.1 | 22 |
| 7470 | Success in Making Zn^{+} from Atomic Zn^0 Encapsulated in an MFI-Type Zeolite with UV Light Irradiation. <i>Journal of the American Chemical Society</i> , 2013, 135, 18481-18489. | 6.6 | 30 |
| 7471 | Theoretical Study on the Mechanism of Palladium-Catalyzed Dearomatization Reaction of Chloromethylnaphthalene. <i>Organometallics</i> , 2013, 32, 52-62. | 1.1 | 14 |
| 7472 | Assessment and Validation of Density Functional Approximations for Iron Carbide and Iron Carbide Cation. <i>Journal of Physical Chemistry A</i> , 2013, 117, 169-173. | 1.1 | 23 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7473 | Quantum Mechanical/Molecular Mechanical Study on the Enantioselectivity of the Enzymatic Baeyer-Villiger Reaction of 4-Hydroxycyclohexanone. <i>Journal of Physical Chemistry B</i> , 2013, 117, 4993-5001. | 1.2 | 31 |
| 7474 | Monohafnium Oxide Clusters HfO_n and HfO_n ($n = 1-6$): Oxygen Radicals, Superoxides, Peroxides, Diradicals, and Triradicals. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1042-1052. | 1.1 | 23 |
| 7475 | Naphthalene dimer and naphthalene dimer with Ar: calibration calculations and the effect of Ar on the stability and vibrational frequencies. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1. | 0.5 | 6 |
| 7476 | Conformational and NMR study of some furan derivatives by DFT methods. <i>Journal of Molecular Modeling</i> , 2013, 19, 4591-4601. | 0.8 | 1 |
| 7477 | Application of recent double-hybrid density functionals to low-lying singlet-singlet excitation energies of large organic compounds. <i>Journal of Chemical Physics</i> , 2013, 139, 164104. | 1.2 | 41 |
| 7478 | Elucidating Band-Selective Sensitization in Iron(II) Polypyridine- TiO_2 Assemblies. <i>Inorganic Chemistry</i> , 2013, 52, 8621-8628. | 1.9 | 48 |
| 7479 | Comprehensive Computational Study of Decamethylzincocene Formation. 1. Reaction of ZnR_2 Reagents with Decamethylzincocene. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4657-4663. | 1.1 | 3 |
| 7480 | Triple Shifts and Thioether Assistance in Rearrangements Associated with an Unusual Biomethylation of the Sterol Side Chain. <i>Journal of Organic Chemistry</i> , 2013, 78, 935-941. | 1.7 | 12 |
| 7481 | Computational Prediction of One-Electron Reduction Potentials and Acid Dissociation Constants for Guanine Oxidation Intermediates and Products. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9518-9531. | 1.2 | 43 |
| 7482 | Internally versus Externally Solvated Derivatives of Doubly Bridged 1,4-Dithio-2-butene: Structures and Dynamic Behavior. A π -Shaped Dimeric Cluster in the Solid State. <i>Journal of Organic Chemistry</i> , 2013, 78, 1149-1156. | 1.7 | 3 |
| 7483 | Comprehensive Computational Study of Decamethylzincocene Formation. 2. Reaction of KH/ZnCl_2 with Decamethylzincocene. <i>Journal of Physical Chemistry A</i> , 2013, 117, 13161-13165. | 1.1 | 1 |
| 7484 | Theoretical Investigation of the Electronic Structure of Fe(II) Complexes at Spin-State Transitions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 509-519. | 2.3 | 85 |
| 7485 | Oxidation Mechanism of $\text{Si}(111)-7 \times 7$ by Water: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 15763-15772. | 1.5 | 4 |
| 7486 | Appropriate description of intermolecular interactions in the methane hydrates: An assessment of DFT methods. <i>Journal of Computational Chemistry</i> , 2013, 34, 121-131. | 1.5 | 111 |
| 7487 | Quantum chemistry studies of adenosine 2503 methylation by S-adenosylmethionine-dependent enzymes. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1409-1415. | 1.0 | 2 |
| 7488 | Synthesis, Structure, and Characterization of Dinuclear Copper(I) Halide Complexes with P ^N Ligands Featuring Exciting Photoluminescence Properties. <i>Inorganic Chemistry</i> , 2013, 52, 2292-2305. | 1.9 | 311 |
| 7489 | Partial atomic charges and their impact on the free energy of solvation. <i>Journal of Computational Chemistry</i> , 2013, 34, 187-197. | 1.5 | 60 |
| 7490 | Electronic, optical, and charge transfer properties of donor-bridge-acceptor hydrazone sensitizers. <i>Structural Chemistry</i> , 2013, 24, 499-506. | 1.0 | 32 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7491 | C ₆₀ and B ₈₀ : A Comparative Study of the Jahn-Teller Effect. <i>Journal of Physics: Conference Series</i> , 2013, 428, 012005. | 0.3 | 3 |
| 7492 | Resonance Raman spectra of <i>ortho</i> -nitrophenol calculated by real-time time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2013, 138, 044101. | 1.2 | 24 |
| 7493 | On-the-fly semiclassical study of internal conversion rates of formaldehyde. <i>Journal of Chemical Physics</i> , 2013, 139, 154311. | 1.2 | 23 |
| 7494 | A comparison of geometric parameters from PBE-based doubly hybrid density functionals PBE0-DH, PBE0-2, and xDH-PBE0. <i>Journal of Chemical Physics</i> , 2013, 139, 174106. | 1.2 | 32 |
| 7495 | Semilocal and hybrid meta-generalized gradient approximations based on the understanding of the kinetic-energy-density dependence. <i>Journal of Chemical Physics</i> , 2013, 138, 044113. | 1.2 | 164 |
| 7496 | Broken symmetry approach to density functional calculation of zero field splittings including anisotropic exchange interactions. <i>Journal of Chemical Physics</i> , 2013, 139, 184110. | 1.2 | 23 |
| 7497 | Melting of γ -Al ₂ O ₃ and vitrification of the undercooled alumina liquid: <i>Ab initio</i> vibrational calculations and their thermodynamic implications. <i>Journal of Chemical Physics</i> , 2013, 138, 064507. | 1.2 | 20 |
| 7498 | Useful lower limits to polarization contributions to intermolecular interactions using a minimal basis of localized orthogonal orbitals: Theory and analysis of the water dimer. <i>Journal of Chemical Physics</i> , 2013, 138, 084102. | 1.2 | 38 |
| 7499 | Nuclear spin-spin coupling in a van der Waals-bonded system: Xenon dimer. <i>Journal of Chemical Physics</i> , 2013, 138, 104313. | 1.2 | 13 |
| 7500 | Multidimensional x-ray spectroscopy of valence and core excitations in cysteine. <i>Journal of Chemical Physics</i> , 2013, 138, 144303. | 1.2 | 23 |
| 7501 | Communication: Nuclear quadrupole moment-induced Cotton-Mouton effect in noble gas atoms. <i>Journal of Chemical Physics</i> , 2013, 139, 181102. | 1.2 | 13 |
| 7502 | Linear-scaling calculation of Hartree-Fock exchange energy with non-orthogonal generalised Wannier functions. <i>Journal of Chemical Physics</i> , 2013, 139, 214103. | 1.2 | 25 |
| 7503 | Flexible nuclear screening approximation to the two-electron spin-orbit coupling based on <i>ab initio</i> parameterization. <i>Journal of Chemical Physics</i> , 2013, 139, 204106. | 1.2 | 8 |
| 7504 | Computational screening study towards redox-active metal-organic frameworks. <i>New Journal of Physics</i> , 2013, 15, 115004. | 1.2 | 13 |
| 7505 | Microbial hydrogen splitting in the presence of oxygen. <i>Biochemical Society Transactions</i> , 2013, 41, 1317-1324. | 1.6 | 2 |
| 7506 | Investigation of TiO ₂ Surface Modification with [6,6]-Phenyl-C ₆₁ -butyric Acid for Titania/Polymer Hybrid Solar Cells. <i>Japanese Journal of Applied Physics</i> , 2013, 52, 112301. | 0.8 | 4 |
| 7507 | Combined crossed beam and theoretical studies of the C(1D) + CH ₄ reaction. <i>Journal of Chemical Physics</i> , 2013, 138, 024311. | 1.2 | 40 |
| 7508 | Experimental and Theoretical Study of Reactions between Manganese Oxide Cluster Cations and Hydrogen Sulfide. <i>Chinese Journal of Chemical Physics</i> , 2013, 26, 679-679. | 0.6 | 7 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7509 | Electron density distribution in tetralithium hypodiphosphate hexahydrate, $\text{Li}_4\text{P}_2\text{O}_6 \cdot 6\text{H}_2\text{O}$. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2013, 69, 344-355. | 0.5 | 12 |
| 7510 | Theoretical Aspects of Hydrolysis of Peptide Bonds by Zinc Metalloenzymes. Chemistry - A European Journal, 2013, 19, 16634-16645. | 1.7 | 13 |
| 7511 | Vibrational solvatochromism: Towards systematic approach to modeling solvation phenomena. Journal of Chemical Physics, 2013, 139, 044111. | 1.2 | 34 |
| 7512 | The Oxidative Mechanism in Electrophilic $\text{C}\ddot{\text{I}}\text{H}$ Activation: The Case of CH_2F_2 and CH_2Cl_2 . Chemistry - an Asian Journal, 2013, 8, 588-595. | 1.7 | 5 |
| 7513 | Nonlinear light scattering in molecules triggered by an impulsive x-ray Raman process. Physical Review A, 2013, 87, 53826. | 1.0 | 9 |
| 7514 | CIDNP as a tool for rapid rearrangements: New insights into cyclobutanoid π -electron radical cations. Journal of Physical Organic Chemistry, 2013, 26, 737-741. | 0.9 | 6 |
| 7515 | Reactivity of Fluoro-Substituted Bis(thiocarbonyl) Donors with Diiodine: An XRD, FT-Raman, and DFT Investigation. Chemistry - an Asian Journal, 2013, 8, 3071-3078. | 1.7 | 8 |
| 7516 | Lowest triplet (n, π^*) state of 2-cyclohexen-1-one: Characterization by cavity ringdown spectroscopy and quantum-chemical calculations. Journal of Chemical Physics, 2013, 139, 214311. | 1.2 | 2 |
| 7517 | Electronic states of thiophene/phenylene co-oligomers: Extreme-ultra violet excited photoelectron spectroscopy observations and density functional theory calculations. Journal of Applied Physics, 2013, 113, 083710. | 1.1 | 14 |
| 7518 | Stable $[\text{M}_2\text{F}_{11}]$ - ($\text{M} = \text{Nb}, \text{Ta}$) Salts of Protonated 1,3-Dimethoxybenzene. European Journal of Inorganic Chemistry, 2013, 2013, 5755-5761. | 1.0 | 20 |
| 7519 | Catalytic Mechanism of Cytochrome P450 2D6 for 4-Hydroxylation of Aripiprazole: A QM/MM Study. Chinese Journal of Chemistry, 2013, 31, 1219-1227. | 2.6 | 12 |
| 7520 | Efficient distance-including integral screening in linear-scaling Møller-Plesset perturbation theory. Journal of Chemical Physics, 2013, 138, 014101. | 1.2 | 66 |
| 7521 | <i>In-Silico</i> Calculations as a Helpful Tool for Designing New Extractants in Liquid-Liquid Extraction. Solvent Extraction and Ion Exchange, 2013, 31, 499-518. | 0.8 | 5 |
| 7522 | Magnetic, electronic, and vibrational properties of metal and fluorinated metal phthalocyanines. Physical Review B, 2013, 87, . | 1.1 | 37 |
| 7523 | The Asymmetry of $(\hat{\alpha})$ -Pinene as Revealed from its Raman Optical Activity Spectrum. Chirality, 2013, 25, 600-605. | 1.3 | 5 |
| 7524 | Structure-Property Relationships of Fe_4S_4 Clusters. ChemPlusChem, 2013, 78, 1082-1098. | 1.3 | 17 |
| 7525 | Tautomeric populations of the charged species of 1,12-diamino-3,6,9-triazadodecane (SpmTrien) studied with computer simulations and cluster expansions. Journal of Physical Organic Chemistry, 2013, 26, 360-366. | 0.9 | 2 |
| 7526 | Linearity condition for orbital energies in density functional theory (III): Benchmark of total energies. Journal of Computational Chemistry, 2013, 34, 1218-1225. | 1.5 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7527 | Structure and vibrational spectra of gauche- and trans-conformers of ethanol: Nonempirical anharmonic calculations and FTIR spectra in argon matrices. <i>Low Temperature Physics</i> , 2013, 39, 389-400. | 0.2 | 24 |
| 7528 | Pharmacophore modelling and electronic feature analysis of hydroxamic acid derivatives, the HIV integrase inhibitors. <i>SAR and QSAR in Environmental Research</i> , 2013, 24, 753-771. | 1.0 | 8 |
| 7529 | Signature of aromatic carbons in the terahertz spectroscopy of bio-chars. , 2013, , . | | 1 |
| 7530 | Watching energy transfer in metalloporphyrin heterodimers using stimulated X-ray Raman spectroscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 15597-15601. | 3.3 | 42 |
| 7531 | On the interactions between poly(ethylene oxide) and graphite oxide: A comparative study by different computational methods. <i>Journal of Chemical Physics</i> , 2013, 138, 094308. | 1.2 | 7 |
| 7532 | Siâ€¦â€¦â€¦H Interligand Interactions in Cobalt(V) and Iridium(V) Bis(silyl)bis(hydride) Complexes. <i>ChemPlusChem</i> , 2013, 78, 1073-1081. | 1.3 | 3 |
| 7533 | Electronic and bonding properties of mono-ruthenium-substituted Keggin-type polyoxometalates: a theoretical study of $[PW_{11}O_{39}Ru]^{n-}(L)$ ($L = Tj ETQq0 0 0 rgBT /Qverlock 10$) | 0.8 | 4 |
| 7534 | Valence excitation energies of alkenes, carbonyl compounds, and azabenzenes by time-dependent density functional theory: Linear response of the ground state compared to collinear and noncollinear spin-flip TDDFT with the Tamm-Dancoff approximation. <i>Journal of Chemical Physics</i> , 2013, 138, 134111. | 1.2 | 62 |
| 7535 | The Mechanism of the Amidases. <i>Journal of Biological Chemistry</i> , 2013, 288, 28514-28523. | 1.6 | 28 |
| 7536 | Stable Aniliny Radical Coordinated to Nickel: X-ray Crystal Structure and Characterization. <i>Chemistry - A European Journal</i> , 2013, 19, 16707-16721. | 1.7 | 30 |
| 7537 | DENSITY FUNCTIONAL STUDY OF THE EFFECTS OF THE SUBSTITUENTS ON THE CHEMICAL REACTIVITY OF THE INDIGO MOLECULE. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350013. | 1.8 | 8 |
| 7538 | Minimum energy pathways via quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2013, 138, 084109. | 1.2 | 14 |
| 7539 | Stereochemical inversion in difunctionalised pillar[5]arenes. <i>Supramolecular Chemistry</i> , 2013, 25, 596-608. | 1.5 | 32 |
| 7540 | COMPARATIVE INVESTIGATION OF THE EFFECT OF TYPE OF DENSITY FUNCTIONAL IN THE DETERMINATION OF GEOMETRICAL PARAMETERS IN A Cu COMPLEX. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350066. | 1.8 | 2 |
| 7541 | Double-core excitations in formamide can be probed by X-ray double-quantum-coherence spectroscopy. <i>Journal of Chemical Physics</i> , 2013, 138, 144301. | 1.2 | 17 |
| 7542 | Functional derivatives of meta-generalized gradient approximation (meta-GGA) type exchange-correlation density functionals. <i>Journal of Chemical Physics</i> , 2013, 138, 244108. | 1.2 | 31 |
| 7543 | Selective Activation of C-Cl and C-F Bonds by SO_3^+ Radical Cations: An Experimental and Computational Study. <i>ChemPlusChem</i> , 2013, 78, 1065-1072. | 1.3 | 7 |
| 7544 | A simplified Tamm-Dancoff density functional approach for the electronic excitation spectra of very large molecules. <i>Journal of Chemical Physics</i> , 2013, 138, 244104. | 1.2 | 242 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7545 | Orbital optimized double-hybrid density functionals. Journal of Chemical Physics, 2013, 139, 024110. | 1.2 | 67 |
| 7546 | Conformational preferences for some 3,3-bis[(4- ϵ^2 -substituted phenylsulfanyl)]-1-methyl-2-piperidinones through spectroscopic and theoretical studies. Journal of Sulfur Chemistry, 2013, 34, 617-626. | 1.0 | 3 |
| 7547 | Ab initio calculation of the deprotonation constants of an atomistically defined nanometer-sized, aluminium hydroxide oligomer. Molecular Simulation, 2013, 39, 220-227. | 0.9 | 1 |
| 7548 | Theoretical Study on the Mechanism of Dioxygen Evolution in Photosystem II. I. Molecular and Electronic Structures at the S ₀ , S ₁ , and S ₂ States of Oxygen-Evolving Complex. Bulletin of the Chemical Society of Japan, 2013, 86, 479-491. | 2.0 | 4 |
| 7549 | Automatic Baseline Correction of Vibrational Circular Dichroism Spectra. Applied Spectroscopy, 2013, 67, 1117-1126. | 1.2 | 1 |
| 7550 | Long-Lived Radical Cation Salts Obtained by Interaction of Monocyclic Arenes with Niobium and Tantalum Pentahalides at Room Temperature: EPR and DFT Studies. Chemistry - A European Journal, 2013, 19, 13962-13969. | 1.7 | 25 |
| 7552 | Multi-Faceted Reactivity of Alkyltellurophenols Towards Peroxyl Radicals: Catalytic Antioxidant Versus Thiol-Depletion Effect. Chemistry - A European Journal, 2013, 19, 7510-7522. | 1.7 | 62 |
| 7554 | Computational Study of Cage Like (ZnO) ₁₂ Cluster Using Hybrid and Hybrid Meta Functionals. Journal of the Chinese Chemical Society, 2013, 60, 1082-1091. | 0.8 | 6 |
| 7555 | A Novel Approach to the Detection and Characterization of PAH Cations and PAH-Photoproducts. Proceedings of the International Astronomical Union, 2013, 9, 286-290. | 0.0 | 4 |
| 7556 | 1,1-Carboboration of Dialkynyltin Compounds using Tri-Organoboranes of Greatly Different Lewis Acid Strength. 1,4-Stannabora-cyclohexa-2,5-dienes and Characterization of Zwitterionic Intermediates. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 1205-1213. | 0.6 | 14 |
| 7557 | Dispersion-Driven Conformational Isomerism in π -Bonded Dimers of Larger Acenes. Angewandte Chemie - International Edition, 2013, 52, 10892-10895. | 7.2 | 47 |
| 7558 | Extracting the hybrid functional mixing parameter from a <i>GW</i> quasiparticle approach. Physica Status Solidi (B): Basic Research, 2013, 250, 1449-1452. | 0.7 | 2 |
| 7559 | Bis(sulfonylimide)ruthenium(VI) Porphyrins: X-ray Crystal Structure and Mechanism of C-H Bond Amination by Density Functional Theory Calculations. Chemistry - A European Journal, 2013, 19, 11320-11331. | 1.7 | 40 |
| 7560 | Tungsten Redox Waves in [XMW ₁₁ O ₄₀] ⁿ⁻ (X = P, Si, Al and Tj) of Inorganic Chemistry, 2013, 2013, 1910-1916. | 1.0 | 19 |
| 7561 | Gold(I) and Silver(I) Complexes of Diphosphacyclobutadiene Cobaltate Sandwich Anions. Chemistry - A European Journal, 2013, 19, 2356-2369. | 1.7 | 23 |
| 7562 | Description of electronic excited states using electron correlation operator. Journal of Chemical Physics, 2013, 139, 104111. | 1.2 | 5 |
| 7563 | Interaction of selected gases with zinc phthalocyanine thin films: theoretical and experimental studies. EPJ Applied Physics, 2013, 64, 10202. | 0.3 | 8 |
| 7564 | Stardust silicate nucleation kick-started by SiO ₂ +TiO ₂ . Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2013, 371, 20110580. | 1.6 | 19 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7565 | Complete π - π^* intramolecular aromatic hydroxylation mechanism through O ₂ activation by a Schiff base macrocyclic dicopper(I) complex. <i>Beilstein Journal of Organic Chemistry</i> , 2013, 9, 585-593. | 1.3 | 6 |
| 7566 | AN EXPERIMENTAL AND THEORETICAL STUDY ON IMIDAZOLIUM-BASED IONIC LIQUID PROMOTED CHLOROMETHYLATION OF AROMATIC HYDROCARBONS. <i>Journal of the Chilean Chemical Society</i> , 2013, 58, 2196-2199. | 0.5 | 4 |
| 7567 | A new family of four-ring bent-core nematic liquid crystals with highly polar transverse and end groups. <i>Beilstein Journal of Organic Chemistry</i> , 2013, 9, 26-35. | 1.3 | 16 |
| 7568 | Mapping Enzymatic Catalysis Using the Effective Fragment Molecular Orbital Method: Towards all ab initio Biochemistry. <i>PLoS ONE</i> , 2013, 8, e60602. | 1.1 | 33 |
| 7569 | Molecular Dynamics Study of Zn(A ⁺) and Zn(A ⁺) ₂ . <i>PLoS ONE</i> , 2013, 8, e70681. | 1.1 | 50 |
| 7570 | OptZyme: Computational Enzyme Redesign Using Transition State Analogues. <i>PLoS ONE</i> , 2013, 8, e75358. | 1.1 | 22 |
| 7571 | Computational study of the rate constants and free energies of intramolecular radical addition to substituted anilines. <i>Beilstein Journal of Organic Chemistry</i> , 2013, 9, 1620-1629. | 1.3 | 27 |
| 7572 | Spectroscopic and Theoretical Studies of Some 3-(4-Substituted phenylsulfanyl)-1-methyl-2-piperidones. <i>Molecules</i> , 2013, 18, 7492-7509. | 1.7 | 5 |
| 7573 | Benchmark Study on the Smallest Bimolecular Nucleophilic Substitution Reaction: H ⁺ +CH ₄ \rightarrow CH ₄ +H ⁺ . <i>Molecules</i> , 2013, 18, 7726-7738. | 1.7 | 2 |
| 7574 | Computational engineering of low bandgap copolymers. <i>Frontiers in Chemistry</i> , 2013, 1, 35. | 1.8 | 59 |
| 7575 | Structure and Stability of Chemically Modified DNA Bases: Quantum Chemical Calculations on 16 Isomers of Diphosphocytosine. , 2013, 2013, 1-10. | | 3 |
| 7576 | Preparation of the Inclusion Complex-Type Nonlinear Optical Polymer. <i>Journal of Spectroscopy</i> , 2013, 2013, 1-7. | 0.6 | 0 |
| 7577 | Host-guest complexes of mixed glycol-bipyridine cryptands: prediction of ion selectivity by quantum chemical calculations, part V. <i>Beilstein Journal of Organic Chemistry</i> , 2013, 9, 1252-1268. | 1.3 | 18 |
| 7579 | An Ab initio Study on the Convergence of Electronic Properties of SiC Nanotubes. <i>Himalayan Physics</i> , 2013, 3, 69-73. | 0.3 | 0 |
| 7580 | Effect of the length of alkyl side chains in the electronic structure of conjugated polymers. <i>Materials Research</i> , 2014, 17, 1369-1374. | 0.6 | 23 |
| 7581 | SERS and DFT study of copper surfaces coated with corrosion inhibitor. <i>Beilstein Journal of Nanotechnology</i> , 2014, 5, 2489-2497. | 1.5 | 45 |
| 7582 | Terahertz Absorption Spectroscopy of Benzamide, Acrylamide, Caprolactam, Salicylamide, and Sulfanilamide in the Solid State. <i>Journal of Spectroscopy</i> , 2014, 2014, 1-9. | 0.6 | 6 |
| 7583 | Quantum Calculation for Musk Molecules Infrared Spectra towards the Understanding of Odor. <i>Advances in Chemistry</i> , 2014, 2014, 1-13. | 1.1 | 1 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7584 | Understanding the Polar Character Trend in a Series of Diels-Alder Reactions Using Molecular Quantum Similarity and Chemical Reactivity Descriptors. <i>Journal of Quantum Chemistry</i> , 2014, 2014, 1-19. | 0.6 | 11 |
| 7585 | Rapid pseudo five-component synthesis of intensively blue luminescent 2,5-di(hetero)arylfurans via a Sonogashira-Glaser cyclization sequence. <i>Beilstein Journal of Organic Chemistry</i> , 2014, 10, 672-679. | 1.3 | 14 |
| 7586 | Optimizing the Structure of Tetracyanoplatinate (II): A Comparison of Relativistic Density Functional Theory Methods. <i>Current Inorganic Chemistry</i> , 2014, 3, 213-219. | 0.2 | 7 |
| 7587 | One-pot three-component synthesis and photophysical characteristics of novel triene merocyanines. <i>Beilstein Journal of Organic Chemistry</i> , 2014, 10, 599-612. | 1.3 | 13 |
| 7588 | Lanczos-driven coupled-cluster damped linear response theory for molecules in polarizable environments. <i>Journal of Chemical Physics</i> , 2014, 141, 244107. | 1.2 | 19 |
| 7589 | X-Ray, IR, NMR, UV-visible spectra and DFT analysis of 5-aryloxy-(1H)-tetrazoles, structure, conformation and tautomerism. <i>Current Chemistry Letters</i> , 2014, 3, 85-96. | 0.5 | 2 |
| 7590 | Total Synthesis of Hybocarpone, a Cytotoxic Naphthazarin Derivative from the Lichen <i>Lecanora hybocarpa</i> , and Related Compounds. <i>Natural Product Communications</i> , 2014, 9, 1934578X1400901. | 0.2 | 2 |
| 7591 | Theoretical Study on Dissociation Mechanisms of Di-ethyl Berylliums and Di- <i>t</i> -butyl Berylliums. <i>Chinese Journal of Chemical Physics</i> , 2014, 27, 168-174. | 0.6 | 1 |
| 7592 | Hybrid Density Functional Study on Plutonium Dioxide. , 2014, , . | | 2 |
| 7593 | Conformations and Metal Ion Affinities of Glutamine Binding with Alkali and Alkaline Earth Metal Cations: an <i>ab initio</i> Study. <i>Chinese Journal of Chemical Physics</i> , 2014, 27, 189-199. | 0.6 | 1 |
| 7594 | Understanding the effects of the number of pyrazines and their positions on charge-transport properties in silylethynylated N-heteropentacenes. <i>Journal of Molecular Modeling</i> , 2014, 20, 2502. | 0.8 | 4 |
| 7595 | Computational study of the complexation of metals ions with poly(amidoamine) PAMAM GO dendrimers. <i>Chemical Physics Letters</i> , 2014, 616-617, 171-177. | 1.2 | 16 |
| 7596 | Solvent effect on characteristic vibration of IR spectrum of 4,4'-dibromodiphenyl ether. <i>Chemical Research in Chinese Universities</i> , 2014, 30, 997-1004. | 1.3 | 4 |
| 7597 | How strongly are the magnetic anisotropy and coordination numbers correlated in lanthanide based molecular magnets?. <i>Journal of Chemical Sciences</i> , 2014, 126, 1569-1579. | 0.7 | 29 |
| 7598 | EFFECT OF THIOPHENE IN BITHIAZOLE-BRIDGED SENSITIZERS ON THE PERFORMANCE OF DYE-SENSITIZED SOLAR CELLS. <i>Nano</i> , 2014, 09, 1440009. | 0.5 | 1 |
| 7599 | Influence of push-pull configuration on the electro-optical and charge transport properties of novel naphtho-difuran derivatives: a DFT study. <i>RSC Advances</i> , 2014, 4, 48876-48887. | 1.7 | 21 |
| 7600 | Vibrational Properties of the Isotopomers of the Water Dimer Derived from Experiment and Computations. <i>Australian Journal of Chemistry</i> , 2014, 67, 426. | 0.5 | 20 |
| 7601 | Assessing the performance of commonly used DFT functionals in studying the chemistry of frustrated Lewis pairs. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1350074. | 1.8 | 21 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7602 | An improved approach for predicting the density of azido compounds. <i>Molecular Simulation</i> , 2014, 40, 491-497. | 0.9 | 5 |
| 7603 | Interstellar condensed (icy) amino acids and precursors: theoretical absorption and circular dichroism under UV and soft X-ray irradiation. <i>Monthly Notices of the Royal Astronomical Society</i> , 2014, 440, 494-503. | 1.6 | 7 |
| 7604 | X-ray and DFT calculated structures of 2-(1H-imidazol-1-yl)-1-(2-naphthyl)ethan-1-one N-phenylthiosemicarbazone and 2-(1H-imidazol-1-yl)-1-(2-naphthyl)ethan-1-one N-(4-chlorophenyl)thiosemicarbazone. <i>Crystallography Reports</i> , 2014, 59, 964-968. | 0.1 | 0 |
| 7605 | Observing and predicting the preferential functionalization of metallic or semiconducting single-walled carbon nanotubes. <i>Europhysics Letters</i> , 2014, 107, 67003. | 0.7 | 1 |
| 7606 | Catalytic Hydrocarbon Oxidation by Palladium-bis-NHC-Complexes. <i>Topics in Catalysis</i> , 2014, 57, 1372-1376. | 1.3 | 14 |
| 7607 | Exploration for the potential precursors for zirconium carbide atomic layer deposition via comprehensive computational mechanistic study of the gas phase decomposition of neopentyl zirconium derivatives. <i>Korean Journal of Chemical Engineering</i> , 2014, 31, 2077-2080. | 1.2 | 1 |
| 7608 | Anomalous Appearance of $\hat{1}/2[C(2)=C(3)]$ Frequencies in IR Spectra of 1,4-Naphthoquinone Hydroxy Derivatives. <i>Journal of Applied Spectroscopy</i> , 2014, 81, 553-564. | 0.3 | 4 |
| 7609 | Experimental and Theoretical Determination of the Antioxidant Properties of Aromatic Monoterpenes of Thymol and 2,5,6-Trifluorothymol. <i>International Journal of Food Properties</i> , 2014, 17, 1162-1168. | 1.3 | 13 |
| 7610 | Theoretical study on phthalocynine- Fe -based fluorescent sensors for cyanide anion. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450006. | 1.8 | 9 |
| 7611 | A full picture of enzymatic catalysis by hydroxynitrile lyases from <i>Hevea brasiliensis</i> : protonation dependent reaction steps and residue-gated movement of the substrate and the product. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26864-26875. | 1.3 | 12 |
| 7612 | Atropisomerization in Confined Space; Cucurbiturils as Tools to Determine the Torsional Barrier of Substituted Biphenyls. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 105-110. | 1.2 | 8 |
| 7613 | The dynamics of interconverting D- and E-forms of the HIV-1 integrase N-terminal domain. <i>European Biophysics Journal</i> , 2014, 43, 485-498. | 1.2 | 5 |
| 7614 | Assessment of theoretical procedures for a diverse set of isomerization reactions involving double-bond migration in conjugated dienes. <i>Chemical Physics</i> , 2014, 441, 166-177. | 0.9 | 49 |
| 7615 | Atmospheric Chemistry Modelling of Amine Emissions from Post Combustion CO ₂ Capture Technology. <i>Energy Procedia</i> , 2014, 63, 822-829. | 1.8 | 4 |
| 7616 | Effect of Intramolecular Hydrogen Bonds on the Gas-Phase Basicity of Guanidines. <i>Australian Journal of Chemistry</i> , 2014, 67, 1056. | 0.5 | 7 |
| 7617 | Structural, elastic, electronic and optical properties of various mineral phases of TiO ₂ from first-principles calculations. <i>Physica Scripta</i> , 2014, 89, 075703. | 1.2 | 15 |
| 7618 | Ab initio density matrix renormalization group study of magnetic coupling in dinuclear iron and chromium complexes. <i>Journal of Chemical Physics</i> , 2014, 140, 054303. | 1.2 | 34 |
| 7619 | Liquid-Liquid Extraction of Acids and Water by a Malonamide: I-Anion Specific Effects on the Polar Core Microstructure of the Aggregated Malonamide. <i>Solvent Extraction and Ion Exchange</i> , 2014, 32, 601-619. | 0.8 | 35 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7620 | First Principles Approaches to Spectroscopic Properties of Complex Materials. Topics in Current Chemistry, 2014, , . | 4.0 | 23 |
| 7621 | Gas-phase reaction of ClO^{\bullet} with $\text{CH}_n\text{Cl}_{4-n}$ ($n = 0, 1, 2, 3$) and CX_3H ($X = \text{F}, \text{Cl}$ and Br): Substituent effect from a comparative study. Canadian Journal of Chemistry, 2014, 92, 868-875. | 0.6 | 1 |
| 7622 | Angle resolved photoemission from organic semiconductors: orbital imaging beyond the molecular orbital interpretation. New Journal of Physics, 2014, 16, 103005. | 1.2 | 44 |
| 7623 | First Principles Methods: A Perspective from Quantum Monte Carlo. Entropy, 2014, 16, 287-321. | 1.1 | 33 |
| 7624 | The Utility of 1,5,7-triazabicyclo[4.4.0]dec-5-ene (TBD) as a Hydrogen Bond Acceptor in the Design of Novel Superbasic Guanidines – A Computational Study. Croatica Chemica Acta, 2014, 87, 423-430. | 0.1 | 3 |
| 7625 | Intramolecular stabilization of the silylene center due to the donor-acceptor interaction with a valence-unbonded nitrogen atom. A theoretical consideration. Russian Chemical Bulletin, 2014, 63, 2599-2604. | 0.4 | 0 |
| 7626 | A QM/MM study of the catalytic mechanism of β -1,4-glucan lyase from the red seaweed Gracilariopsis lemaneiformis. RSC Advances, 2014, 4, 54398-54408. | 1.7 | 5 |
| 7627 | A Multiscale Approach to Modelling Drug Metabolism by Membrane-Bound Cytochrome P450 Enzymes. PLoS Computational Biology, 2014, 10, e1003714. | 1.5 | 42 |
| 7628 | GaN doped C60 as a nano bio sensor for the detection of mispairing in adenine-thymine base pair. Main Group Chemistry, 2014, 13, 307-317. | 0.4 | 1 |
| 7629 | Alkylpurine Glycosylase D Employs DNA Sculpting as a Strategy to Extrude and Excise Damaged Bases. PLoS Computational Biology, 2014, 10, e1003704. | 1.5 | 3 |
| 7630 | Assessment of density-functionals for describing the $\text{X}^{\bullet} + \text{CH}_3\text{ONO}_2$ gas-phase reactions with $X = \text{F}, \text{OH}, \text{CH}_2\text{CN}$. Physical Chemistry Chemical Physics, 2014, 16, 26769-26778. | 1.3 | 11 |
| 7631 | 17. Theoretical Approaches to Structure and Spectroscopy of Earth Materials. , 2014, , 691-744. | | 1 |
| 7632 | Nuclear spin circular dichroism in fullerenes: a computational study. Chemical Communications, 2014, 50, 15228-15231. | 2.2 | 9 |
| 7633 | Hirshfeld atom refinement. IUCr, 2014, 1, 361-379. | 1.0 | 200 |
| 7634 | Pyridyl- and Pyridylperoxy Radicals – A Matrix Isolation Study. Australian Journal of Chemistry, 2014, 67, 1324. | 0.5 | 12 |
| 7635 | Studies of the Structure, Amidicity, and Reactivity of N-Chlorohydroxamic Esters and N-Chloro- β,β -dialkylhydrazides: Anomeric Amides with Low Resonance Energies. Australian Journal of Chemistry, 2014, 67, 1344. | 0.5 | 13 |
| 7636 | Many-body exchange-overlap interactions in rare gases and water. Journal of Chemical Physics, 2014, 141, 224106. | 1.2 | 25 |
| 7637 | Self-interaction corrected density functional calculations of Rydberg states of molecular clusters: N,N-dimethylisopropylamine. Journal of Chemical Physics, 2014, 141, 234308. | 1.2 | 22 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7638 | Nuclear spin circular dichroism. <i>Journal of Chemical Physics</i> , 2014, 140, 134103. | 1.2 | 20 |
| 7639 | Probing ground and low-lying excited states for HIO ₂ isomers. <i>Journal of Chemical Physics</i> , 2014, 141, 234303. | 1.2 | 8 |
| 7640 | Three-dimensional attosecond resonant stimulated X-ray Raman spectroscopy of electronic excitations in core-ionized glycine. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24323-24331. | 1.3 | 16 |
| 7641 | Electronic Structure of Covalently Linked Zinc Bacteriochlorin Molecular Arrays: Insights into Molecular Design for NIR Light Harvesting. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9901-9913. | 1.1 | 10 |
| 7642 | Stabilization of Complexes of Redox-Active Guanidino-Functionalized Aromatic Compounds (GFAs) by Hydrogen-Bonding. <i>Australian Journal of Chemistry</i> , 2014, 67, 1044. | 0.5 | 8 |
| 7643 | On the Mechanism of the Palladium Bis(NHC) Complex Catalyzed CH Functionalization of Propane: Experiment and DFT Calculations. <i>Chemistry - A European Journal</i> , 2014, 20, 14872-14879. | 1.7 | 36 |
| 7644 | Hybrid DFT calculation of Fe NMR resonances and orbital order in magnetite. <i>Physical Review B</i> , 2014, 90, . | 1.1 | 8 |
| 7645 | Assessment of amide I spectroscopic maps for a gas-phase peptide using IR-UV double-resonance spectroscopy and density functional theory calculations. <i>Journal of Chemical Physics</i> , 2014, 140, 224111. | 1.2 | 26 |
| 7646 | An insight into the structures, stabilities, and bond character of BnPt ($n=1\text{--}4$) clusters. <i>Journal of Molecular Modeling</i> , 2014, 20, 2482. | 0.8 | 5 |
| 7647 | Time-dependent density-functional theory simulation of electron wave-packet scattering with nanoflakes. <i>Physical Review B</i> , 2014, 90, . | 1.1 | 18 |
| 7648 | Structure-Property Relationships in an Iridium(III) Bis(Terpyridine) Complex with Extended Conjugated Side chains. <i>Journal of Physical Chemistry A</i> , 2014, 118, 12137-12148. | 1.1 | 5 |
| 7650 | Significant Substituent Effect on the Anomerization of Pyranosides: Mechanism of Anomerization and Synthesis of a 1,2- <i>cis</i> Glucosamine Oligomer from the 1,2- <i>trans</i> Anomer. <i>Chemistry - A European Journal</i> , 2014, 20, 124-132. | 1.7 | 21 |
| 7651 | How important is self-consistency for the dDsC density dependent dispersion correction?. <i>Journal of Chemical Physics</i> , 2014, 140, 18A516. | 1.2 | 24 |
| 7652 | Recommending Hartree-Fock Theory with London-Dispersion and Basis-Set-Superposition Corrections for the Optimization or Quantum Refinement of Protein Structures. <i>Journal of Physical Chemistry B</i> , 2014, 118, 14612-14626. | 1.2 | 53 |
| 7653 | Energetics of heterometal substitution in $\text{Keggin} [\text{MO}_4\text{Al}_{12}(\text{OH})_{24}(\text{OH}_2)_{12}]^{6/7/8+}$ ions. <i>American Mineralogist</i> , 2014, 99, 2337-2343. | 0.9 | 7 |
| 7654 | Extreme electric fields power catalysis in the active site of ketosteroid isomerase. <i>Science</i> , 2014, 346, 1510-1514. | 6.0 | 392 |
| 7655 | An improved classical mapping method for homogeneous electron gases at finite temperature. <i>Journal of Chemical Physics</i> , 2014, 141, 064115. | 1.2 | 9 |
| 7656 | Embedded-cluster calculations in a numeric atomic orbital density-functional theory framework. <i>Journal of Chemical Physics</i> , 2014, 141, 024105. | 1.2 | 38 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7657 | Analysis of nonlinear optical properties in donor-acceptor materials. <i>Journal of Chemical Physics</i> , 2014, 140, 184308. | 1.2 | 32 |
| 7658 | A self-interaction-free local hybrid functional: Accurate binding energies vis-à-vis accurate ionization potentials from Kohn-Sham eigenvalues. <i>Journal of Chemical Physics</i> , 2014, 140, 18A510. | 1.2 | 66 |
| 7659 | Relevant Interactions of Antimicrobial Iron Chelators and Membrane Models Revealed by Nuclear Magnetic Resonance and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2014, 118, 14590-14601. | 1.2 | 11 |
| 7660 | All-Atom CHARMM Force Field and Bulk Properties of Perfluorozinc Phthalocyanines. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11583-11590. | 1.1 | 9 |
| 7661 | In Situ Observation of Degradation by Ligand Substitution in Small-Molecule Phosphorescent Organic Light-Emitting Diodes. <i>Chemistry of Materials</i> , 2014, 26, 6578-6584. | 3.2 | 30 |
| 7662 | Binuclear copper(ii) and nickel(ii) complexes based on N,N'-bis(3-formyl-5-tert-butylsalicylidene)-1,3-diaminopropan-2-ol: physicochemical and theoretical study. <i>Russian Chemical Bulletin</i> , 2014, 63, 673-683. | 0.4 | 3 |
| 7663 | A computational study of potential molecular switches that exploit Baird's rule on excited-state aromaticity and antiaromaticity. <i>Faraday Discussions</i> , 2014, 174, 105-124. | 1.6 | 22 |
| 7664 | FOHI-D: An iterative Hirshfeld procedure including atomic dipoles. <i>Journal of Chemical Physics</i> , 2014, 140, 144104. | 1.2 | 14 |
| 7665 | Describing long-range charge-separation processes with subsystem density-functional theory. <i>Journal of Chemical Physics</i> , 2014, 140, 164103. | 1.2 | 39 |
| 7666 | First principles molecular dynamics without self-consistent field optimization. <i>Journal of Chemical Physics</i> , 2014, 140, 044117. | 1.2 | 33 |
| 7667 | TDDFT Assessment of Functionals for Optical $\pi \rightarrow \pi^*$ Transitions in Small Radicals. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11033-11046. | 1.1 | 15 |
| 7668 | Carbon Nitride Photocatalysts for Water Splitting: A Computational Perspective. <i>Journal of Physical Chemistry C</i> , 2014, 118, 24833-24842. | 1.5 | 106 |
| 7669 | A comparative synthetic, magnetic and theoretical study of functional M_4Cl_4 cubane-type Co(ii) and Ni(ii) complexes. <i>Dalton Transactions</i> , 2014, 43, 7847. | 1.6 | 40 |
| 7670 | Epoxyalcohols: Bioactivation and Conjugation Required for Skin Sensitization. <i>Chemical Research in Toxicology</i> , 2014, 27, 1860-1870. | 1.7 | 10 |
| 7671 | Using computational methods to explore improvements to Knölker's iron catalyst. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 4361-4371. | 1.5 | 19 |
| 7672 | Ethylene Trimerisation with Cr-PNP Catalysts: A Theoretical Benchmarking Study and Assessment of Catalyst Oxidation State. <i>Australian Journal of Chemistry</i> , 2014, 67, 1481. | 0.5 | 28 |
| 7673 | Spin-State-Dependent Properties of an Iron(III) Hydrogenase Mimic. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 3587-3599. | 1.0 | 12 |
| 7674 | The chemistry of bowtiene (tricyclo[5.3.0.0 ^{2,6}]decapentaene): a computational study. <i>Canadian Journal of Chemistry</i> , 2014, 92, 378-385. | 0.6 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7675 | Axial Thiophenolate Coordination on Diiron(III)bisporphyrin: Influence of Heme-Heme Interactions on Structure, Function and Electrochemical Properties of the Individual Heme Center. <i>Inorganic Chemistry</i> , 2014, 53, 11925-11936. | 1.9 | 46 |
| 7676 | Synthesis and Characterization of a Stable Copper(I) Complex for Radiopharmaceutical Applications. <i>ChemPlusChem</i> , 2014, 79, 1284-1293. | 1.3 | 9 |
| 7677 | Syntheses and characterization of liposome-incorporated adamantyl aminoguanidines. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 6005-6013. | 1.5 | 10 |
| 7678 | Time-, frequency-, and wavevector-resolved x-ray diffraction from single molecules. <i>Journal of Chemical Physics</i> , 2014, 140, 204311. | 1.2 | 29 |
| 7679 | Shared-memory parallelization of a local correlation multi-reference CI program. <i>Computer Physics Communications</i> , 2014, 185, 3175-3188. | 3.0 | 8 |
| 7680 | HCN exchange on [Cu(HCN) ₄] ⁺ : a quantum chemical investigation. <i>Journal of Coordination Chemistry</i> , 2014, 67, 2185-2194. | 0.8 | 0 |
| 7681 | Influence of the environment on protein bond energies. <i>Chemical Physics Letters</i> , 2014, 615, 75-82. | 1.2 | 0 |
| 7682 | Reactivity of low-oxidation state tin compounds: an overview of the benefits of combining DFT Theory and experimental NMR spectroscopy. <i>Canadian Journal of Chemistry</i> , 2014, 92, 447-461. | 0.6 | 1 |
| 7683 | Synthesis and Characterization of Spirosilanes - 1,2-Hydroboration and 1,1-Carboboration. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 3411-3419. | 1.0 | 6 |
| 7684 | Structural Evolution of Homoleptic Heterodinuclear Copper-Nickel Carbonyl Anions Revealed Using Photoelectron Velocity-Map Imaging. <i>Inorganic Chemistry</i> , 2014, 53, 10909-10916. | 1.9 | 24 |
| 7685 | Activation Barriers of Oxygen Transformation at the Active Site of [FeFe] Hydrogenases. <i>Inorganic Chemistry</i> , 2014, 53, 11890-11902. | 1.9 | 22 |
| 7686 | Spectroscopic Investigation of the Wettability of Multilayer Graphene Using Highly Ordered Pyrolytic Graphite as a Model Material. <i>Langmuir</i> , 2014, 30, 12827-12836. | 1.6 | 81 |
| 7687 | Quantum chemical investigation of the primary thermal pyrolysis reactions of the sodium carboxylate group in a brown coal model. <i>Journal of Molecular Modeling</i> , 2014, 20, 2523. | 0.8 | 3 |
| 7688 | Behavior of Highly Diluted Electrolytes in Strong Electric Fields - Prevention of Alumina Deposition on Grading Electrodes in HVDC Transmission Modules by CO ₂ -induced pH-Control. <i>Chemistry - A European Journal</i> , 2014, 20, 12091-12103. | 1.7 | 15 |
| 7689 | The Buildup of Eight-Vertex Tetrametallaborane Clusters: Bisdisphenoidal versus Tetracapped Tetrahedral Structures. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 3614-3618. | 1.0 | 1 |
| 7690 | Solid-State NMR Characterization of Paramagnetic Bis(L-valinato)copper(II) Stereoisomers - Effect of Conformational Disorder and Molecular Mobility on ¹³ C and ² H Fast Magic-Angle Spinning Spectra. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 3330-3340. | 1.0 | 9 |
| 7691 | Nuclear quadrupole moment-induced Cotton-Mouton effect in molecules. <i>Journal of Chemical Physics</i> , 2014, 140, 024103. | 1.2 | 11 |
| 7692 | Evaluating interaction energies of weakly bonded systems using the Buckingham-Hirshfeld method. <i>Journal of Chemical Physics</i> , 2014, 140, 184105. | 1.2 | 5 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7693 | Perturbative treatment of anharmonic vibrational effects on bond distances: An extended langevin dynamics method. <i>Journal of Computational Chemistry</i> , 2014, 35, 467-478. | 1.5 | 1 |
| 7694 | Understanding Polymorphism in Organic Semiconductor Thin Films through Nanoconfinement. <i>Journal of the American Chemical Society</i> , 2014, 136, 17046-17057. | 6.6 | 179 |
| 7695 | Common Physical Framework Explains Phase Behavior and Dynamics of Atomic, Molecular, and Polymeric Network Formers. <i>Physical Review X</i> , 2014, 4, . | 2.8 | 16 |
| 7696 | Kinetics of radical-molecule reactions in aqueous solution: A benchmark study of the performance of density functional methods. <i>Journal of Computational Chemistry</i> , 2014, 35, 2019-2026. | 1.5 | 211 |
| 7697 | Testing time-dependent density functional theory with depopulated molecular orbitals for predicting electronic excitation energies of valence, Rydberg, and charge-transfer states and potential energies near a conical intersection. <i>Journal of Chemical Physics</i> , 2014, 141, 104106. | 1.2 | 13 |
| 7698 | Communication: Double-hybrid functionals from adiabatic-connection: The QIDH model. <i>Journal of Chemical Physics</i> , 2014, 141, 031101. | 1.2 | 154 |
| 7699 | Liquid-crystalline structure-property relationships in halogen-terminated derivatives of cyanobiphenyl. <i>Liquid Crystals</i> , 2014, 41, 1635-1646. | 0.9 | 28 |
| 7700 | The one-electron oxidation of a dithiolate molecule: The importance of chemical intuition. <i>Journal of Chemical Physics</i> , 2014, 140, 18A519. | 1.2 | 8 |
| 7701 | On the Concept of Hemilability: Insights into a Donor-Functionalized Iridium(I) NHC Motif and Its Impact on Reactivity. <i>Inorganic Chemistry</i> , 2014, 53, 12767-12777. | 1.9 | 46 |
| 7703 | Mixed Ligand Cu ^{II} N ₂ O ₂ Complexes: Biomimetic Synthesis, Activities in Vitro and Biological Models, Theoretical Calculations. <i>Inorganic Chemistry</i> , 2014, 53, 13019-13030. | 1.9 | 15 |
| 7704 | Excited states of OH-(H ₂ O) _n clusters for n = 1-4: An <i>ab initio</i> study. <i>Journal of Chemical Physics</i> , 2014, 141, 104315. | 1.2 | 18 |
| 7705 | Unusual crystal structure of <i>N</i> -substituted maleamic acid - very strong effect of intramolecular hydrogen bonds. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2014, 70, 942-947. | 0.5 | 2 |
| 7706 | Toward a Unified Model of Passive Drug Permeation II: The Physicochemical Determinants of Unbound Tissue Distribution with Applications to the Design of Hepatoselective Glucokinase Activators. <i>Drug Metabolism and Disposition</i> , 2014, 42, 1599-1610. | 1.7 | 19 |
| 7707 | Coupled-cluster reaction barriers of : An application of the coupled-cluster/Kohn-Sham density functional theory model chemistry. <i>Journal of Computational Chemistry</i> , 2014, 35, 507-517. | 1.5 | 20 |
| 7708 | Synthesis and Characterization of a Uranium(II) Monoarene Complex Supported by σ -Backbonding. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 7158-7162. | 7.2 | 172 |
| 7709 | A little spin on the side: solvent and temperature dependent paramagnetism in [RuII(bpy) ₂ (phendione)] ²⁺ . <i>Dalton Transactions</i> , 2014, 43, 17729-17739. | 1.6 | 7 |
| 7710 | 1,3,2-Diselena- and 1,3,2-Ditelluraphospholanes with an Annelated 1,2-Dicarba-closo-dodecaborane(12) Unit. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 1929-1948. | 1.0 | 7 |
| 7711 | Synthesis of ϵ -cyclopentene derivatives using 1,2-hydroboration, 1,1-organoboration and protodeborylation. <i>Applied Organometallic Chemistry</i> , 2014, 28, 280-285. | 1.7 | 8 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7712 | Accurate density functional theory description of binding constants and NMR chemical shifts of weakly interacting complexes of C ₆₀ with corannulene-based molecular bowls. <i>Journal of Computational Chemistry</i> , 2014, 35, 181-191. | 1.5 | 16 |
| 7713 | Guest–host interaction in an aza crown analog. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 708-719. | 1.0 | 6 |
| 7714 | Hybrid density functional theory study of Cu(In _{1-x} Gax)Se ₂ band structure for solar cell application. <i>AIP Advances</i> , 2014, 4, . | 0.6 | 19 |
| 7715 | Structure and Vibrational Analyses of LiP ₁₅ . <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 5135-5144. | 1.0 | 12 |
| 7716 | Impact of divalent metal cations on the catalysis of peptide bonds: a DFT study. <i>Journal of Coordination Chemistry</i> , 2014, 67, 3920-3931. | 0.8 | 2 |
| 7717 | Theoretical study on S<i>_H</i></sub> </i></sub>2 reaction of methyl radical with three-membered ring. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1594-1601. | 1.0 | 1 |
| 7718 | Detailed Geometric and Electronic Structures of a One-Electron-Oxidized Ni Salophen Complex and Its Amido Derivatives. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 3479-3487. | 1.0 | 19 |
| 7719 | Selective Synthesis of Stannoles by 1,1-Carbaboration of Bis(trimethylsilylethynyl)tin Compounds Using Weakly and Strongly Electrophilic Triorganoboranes: Characterization of a Zwitterionic Intermediate. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 2103-2112. | 1.0 | 16 |
| 7720 | Density functional theory approach to gold-ligand interactions: Separating true effects from artifacts. <i>Journal of Chemical Physics</i> , 2014, 140, 244313. | 1.2 | 14 |
| 7721 | Base-induced 1,3-σ-tropic Rearrangement of Mesitylphosphonium Salts. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 1615-1619. | 1.0 | 6 |
| 7722 | Solvent-free click chemistry for tetrazole synthesis from 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-Based fluorinated ionic liquids, their micellization, and density functional theory studies. <i>RSC Advances</i> , 2014, 4, 64128-64137. | 1.7 | 20 |
| 7723 | HOMO Stabilisation in i-Extended Dibenzotetrathiafulvalene Derivatives for Their Application in Organic Field-Effect Transistors. <i>Chemistry - A European Journal</i> , 2014, 20, 16672-16679. | 1.7 | 14 |
| 7724 | Synthesis and Characterization of Nickel Compounds with Tetradentate Thiolate–Thioether Ligands as Precursors for [NiFe]-Hydrogenase Models. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 148-155. | 1.0 | 5 |
| 7725 | Gradient of molecular Hartree–Fock–Bogoliubov energy with a linear combination of atomic orbital quasiparticle wave functions. <i>Journal of Chemical Physics</i> , 2014, 140, 084115. | 1.2 | 5 |
| 7726 | Geometrical and optical benchmarking of copper(II) guanidine–quinoline complexes: Insights from TD-DFT and many-body perturbation theory (part II). <i>Journal of Computational Chemistry</i> , 2014, 35, 2146-2161. | 1.5 | 31 |
| 7727 | Synthesis, Structure, and Optical Properties of Pt(II) and Pd(II) Complexes with Oxazolyl- and Pyridyl-Functionalized DPPM-Type Ligands: A Combined Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , 2014, 53, 12739-12756. | 1.9 | 8 |
| 7728 | Phosphorescent C–S* Cyclometalated Pt(II) Dibenzofuranyl-NHC Complexes - An Auxiliary Ligand Study. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 256-264. | 1.0 | 45 |
| 7729 | The Oxidation of Sulfur Dioxide by Single and Double Oxygen Transfer Paths. <i>ChemPhysChem</i> , 2014, 15, 2723-2731. | 1.0 | 10 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7730 | Theoretical studies of special relativity in atoms and molecules. <i>Chemical Modelling</i> , 2014, , 88-133. | 0.2 | 0 |
| 7731 | Reaction of Germylene with Sulfur Dioxide: Gas-Phase Kinetic and Theoretical Studies. <i>Organometallics</i> , 2014, 33, 6493-6503. | 1.1 | 6 |
| 7732 | Matrix effect on vibrational frequencies: Experiments and simulations for HCl and HNgCl (Ng = Kr and) Tj ETQq0 0 0 rBT /Overlock 10 T | 1.2 | 21 |
| 7733 | Characterization of multiple fragmentation pathways initiated by collision-induced dissociation of multifunctional anions formed by deprotonation of 2-nitrobenzenesulfonylglycine. <i>Journal of Mass Spectrometry</i> , 2014, 49, 168-177. | 0.7 | 4 |
| 7734 | Phosphorescent Iridium(III) Complexes of Cyclometalated 5-Aryl-1 <i>H</i> -1,2,4-Triazole Ligands: Structural, Computational, Spectroscopic, and Device Studies. <i>Journal of Physical Chemistry C</i> , 2014, 118, 27763-27771. | 1.5 | 18 |
| 7735 | Examination of small molecule losses in 5-methylpyranopelargonidin MS/MS CID spectra by DFT calculations. <i>Journal of Mass Spectrometry</i> , 2014, 49, 1314-1321. | 0.7 | 7 |
| 7736 | Mechanism of Ni N-heterocyclic carbene catalyst for C=O bond hydrogenolysis of diphenyl ether: a density functional study. <i>Dalton Transactions</i> , 2014, 43, 18123-18133. | 1.6 | 40 |
| 7737 | Density Functional Theory Beyond the Generalized Gradient Approximation for Surface Chemistry. <i>Topics in Current Chemistry</i> , 2014, , 25-51. | 4.0 | 9 |
| 7738 | A new efficient method for calculation of Frenkel exciton parameters in molecular aggregates. <i>Journal of Chemical Physics</i> , 2014, 140, 174101. | 1.2 | 20 |
| 7739 | Binding of Mazindol and Analogs to the Human Serotonin and Dopamine Transporters. <i>Molecular Pharmacology</i> , 2014, 85, 208-217. | 1.0 | 22 |
| 7740 | Supramolecular architectures of N,N,N',N'-tetrakis-(2-hydroxyethyl)ethylenediamine and tris(2-hydroxyethyl)amine with La(III) picrate. <i>RSC Advances</i> , 2014, 4, 59248-59264. | 1.7 | 7 |
| 7741 | Energy density functionals from the strong-coupling limit applied to the anions of the He isoelectronic series. <i>Journal of Chemical Physics</i> , 2014, 140, 18A532. | 1.2 | 19 |
| 7742 | Analytic calculations of hyper-Raman spectra from density functional theory hyperpolarizability gradients. <i>Journal of Chemical Physics</i> , 2014, 141, 134107. | 1.2 | 12 |
| 7743 | Release of Cyanopyridine from a Ruthenium Complex Adsorbed on Gold: Surface-Enhanced Raman Scattering, Electrochemistry, and Density Functional Theory Analyses. <i>Journal of Physical Chemistry C</i> , 2014, 118, 27925-27932. | 1.5 | 5 |
| 7744 | Systematic Improvement of Potential-Derived Atomic Multipoles and Redundancy of the Electrostatic Parameter Space. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5493-5504. | 2.3 | 30 |
| 7745 | Antraquinone-Based Intramolecular Charge-Transfer Compounds: Computational Molecular Design, Thermally Activated Delayed Fluorescence, and Highly Efficient Red Electroluminescence. <i>Journal of the American Chemical Society</i> , 2014, 136, 18070-18081. | 6.6 | 822 |
| 7746 | Nuclear-Spin-Induced Cotton-Mouton Effect in a Strong External Magnetic Field. <i>ChemPhysChem</i> , 2014, 15, 2337-2350. | 1.0 | 10 |
| 7747 | Almost Enclosed Buckyball Joints: Synthesis, Complex Formation, and Computational Simulations of Pentypticene-Extended Tribenzotriquinacene. <i>ChemPhysChem</i> , 2014, 15, 3855-3863. | 1.0 | 21 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7748 | Experimental and Theoretical Characterization of 5,10-Diminoporphodimethenes: Dearomatized Porphyrinoids from Palladium-Catalyzed Hydrazinations of 5,10-Diarylporphyrins. <i>ChemPlusChem</i> , 2014, 79, 813-824. | 1.3 | 5 |
| 7749 | Semiconducting Clathrates Meet Gas Hydrates: Xe ₂₄ [Sn ₁₃₆]. <i>Chemistry - A European Journal</i> , 2014, 20, 6693-6698. | 1.7 | 14 |
| 7750 | CO-dynamics in the active site of cytochrome c oxidase. <i>Journal of Chemical Physics</i> , 2014, 140, 145101. | 1.2 | 6 |
| 7751 | The DFT+U/mol method and its application to the adsorption of CO on platinum model clusters. <i>Journal of Chemical Physics</i> , 2014, 140, 174709. | 1.2 | 10 |
| 7752 | The possibility of optical excitations at the smallest gap of Cu-delafoosite nanocrystals. <i>Journal Physics D: Applied Physics</i> , 2014, 47, 405301. | 1.3 | 0 |
| 7753 | Ab initio study of mechanical stability, thermodynamic and elastic properties of Rh, RhH, and RhH ₂ under high temperature and pressure. <i>Journal of Materials Research</i> , 2014, 29, 1334-1343. | 1.2 | 5 |
| 7754 | Theoretical study of hyperfine interactions and optically detected magnetic resonance spectra by simulation of the C ₂₉₁ [NV] ⁻ H ₁₇₂ diamond cluster hosting nitrogen-vacancy center. <i>New Journal of Physics</i> , 2014, 16, 083014. | 1.2 | 23 |
| 7755 | Surface Hopping Dynamics with DFT Excited States. <i>Topics in Current Chemistry</i> , 2014, 368, 415-444. | 4.0 | 53 |
| 7756 | Chemisorption-induced two- to three-dimensions structural transformations in gold pentamer (CO) _n Au ₅ (n = 0-5). <i>Journal of Molecular Modeling</i> , 2014, 20, 2490. | 0.8 | 0 |
| 7757 | A QM/MM study of the associative mechanism for the phosphorylation reaction catalyzed by protein kinase A and its D166A mutant. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 1077-1091. | 1.3 | 11 |
| 7758 | X-ray diffraction, DFT, spectroscopic study and insecticidal activity of (3-cyano-1-(2,6-dichloro-4-(trifluoromethyl)phenyl)-4-((trifluoromethyl)sulfinyl)-1H-pyrazol-5-yl)(2-(triethylammonio)acetate)amide inner salt. <i>Crystallography Reports</i> , 2014, 59, 1078-1083. | 0.0 | 0 |
| 7759 | Excitons in Time-Dependent Density-Functional Theory. <i>Topics in Current Chemistry</i> , 2014, 368, 185-217. | 4.0 | 20 |
| 7760 | A comparative study on the adsorption behaviors of PABA in the silver nano-particles. <i>Journal of Molecular Structure</i> , 2014, 1074, 660-665. | 1.8 | 9 |
| 7761 | Computational insight into Wilkinson's complex catalyzed [2+2] cycloaddition mechanism leading to pyridine formation. <i>Journal of Organometallic Chemistry</i> , 2014, 768, 15-22. | 0.8 | 15 |
| 7762 | Density functional theory study on the interaction of magnesium ions with graphene surface. <i>Japanese Journal of Applied Physics</i> , 2014, 53, 02BD02. | 0.8 | 6 |
| 7763 | Theoretical investigation of geometric configurations and vibrational spectra in citric acid complexes. <i>Materials Research</i> , 2014, 17, 550-556. | 0.6 | 18 |
| 7764 | Microwave Spectroscopy of Biomolecular Building Blocks. <i>Topics in Current Chemistry</i> , 2014, 364, 335-401. | 4.0 | 41 |
| 7765 | 8th Congress on Electronic Structure: Principles and Applications (ESPA 2012). <i>Highlights in Theoretical Chemistry</i> , 2014, , . | 0.0 | 0 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7766 | Description of Bond Pseudorotation, Bond Pseudolibration, and Ring Pseudoinversion Processes Caused by the Pseudo-Jahn-Teller Effect: Fluoro Derivatives of the Cyclopropane Radical Cation. <i>Australian Journal of Chemistry</i> , 2014, 67, 435. | 0.5 | 21 |
| 7767 | Vinylsilylferrocenes and Ethynyl(vinyl)silylferrocenes. Synthesis, Multinuclear Magnetic Resonance Study and DFT Calculations. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2014, 69, 704-714. | 0.3 | 1 |
| 7768 | Multidimensional scattering of attosecond x-ray pulses detected by photon-coincidence. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2014, 47, 124037. | 0.6 | 8 |
| 7769 | Progress on New Approaches to Old Ideas: Orbital-Free Density Functionals. <i>Letters in Mathematical Physics</i> , 2014, , 113-134. | 0.4 | 30 |
| 7770 | Spatial structure of 2-(2-hydroxyphenyl)-4-methylchromanes and some specific features of intramolecular hydrogen bond. <i>Russian Chemical Bulletin</i> , 2014, 63, 1976-1985. | 0.4 | 0 |
| 7771 | DFT study of mechanisms of the antioxidant effect of natural polyhydroxy-1,4-naphthoquinones. Reactions of echinamines A and B, metabolites of sea urchin <i>Scaphechinus mirabilis</i> , with hydroperoxyl radical. <i>Russian Chemical Bulletin</i> , 2014, 63, 1993-1999. | 0.4 | 6 |
| 7772 | 1,2-Hydroboration and 1,1-Carboboration of Alkynyl(ferrocenyl)vinylsilanes. Novel Siloles. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2014, 69, 1269-1289. | 0.3 | 5 |
| 7773 | High-resolution structures of cholesterol oxidase in the reduced state provide insights into redox stabilization. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 3155-3166. | 2.5 | 9 |
| 7774 | Tuning nondoped carbon nanotubes to an efficient metal-free electrocatalyst for oxygen reduction reaction by localizing the orbital of the nanotubes with topological defects. <i>Nanoscale</i> , 2014, 6, 14262-14269. | 2.8 | 41 |
| 7775 | UV-vis spectra of singlet state cationic polycyclic aromatic hydrocarbons: Time-dependent density functional theory study. <i>Journal of Chemical Physics</i> , 2014, 140, 044324. | 1.2 | 6 |
| 7776 | <i>N</i> -Trimethylsilylaminophosphines: Solution-state Structures, Studied by Multinuclear Magnetic Resonance and DFT Methods. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2014, 640, 195-200. | 0.6 | 0 |
| 7777 | Topological isomerism in a chiral handcuff catenane. <i>Chemical Science</i> , 2014, 5, 90-100. | 3.7 | 24 |
| 7778 | New pyrido[3,4-b]pyrazine-based sensitizers for efficient and stable dye-sensitized solar cells. <i>Chemical Science</i> , 2014, 5, 206-214. | 3.7 | 102 |
| 7779 | Burning velocities and kinetics of H ₂ /NF ₃ /N ₂ , CH ₄ /NF ₃ /N ₂ , and C ₃ H ₈ /NF ₃ /N ₂ flames. <i>Combustion and Flame</i> , 2014, 161, 1425-1431. | 2.8 | 9 |
| 7780 | Functionalization of silicon carbide nanotube by dichlorocarbene: A density functional theory study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2014, 56, 377-385. | 1.3 | 7 |
| 7781 | Tautomerism in substituted cyanopyridone: Ultrafast dynamics and TDDFT studies in water. <i>Chemical Physics Letters</i> , 2014, 600, 1-6. | 1.2 | 1 |
| 7782 | Molecular structure of amino alcohols on aluminum surface. <i>Journal of Molecular Structure</i> , 2014, 1063, 51-59. | 1.8 | 11 |
| 7783 | The role of structural CH compared with phenolic OH sites on the antioxidant activity of oleuropein and its derivatives as a great non-flavonoid family of the olive components: A DFT study. <i>Food Chemistry</i> , 2014, 164, 251-258. | 4.2 | 45 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7784 | Experimental and theoretical spectroscopic analysis, HOMO–LUMO, and NBO studies of cyanuric chloride. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 127, 454-462. | 2.0 | 12 |
| 7785 | The reaction of the benzene cation with acetylenes for the growth of PAHs in the interstellar medium. <i>Chemical Physics Letters</i> , 2014, 595-596, 13-19. | 1.2 | 5 |
| 7786 | The Second-Order Polarization Propagator Approximation (SOPPA) method coupled to the polarizable continuum model. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 54-60. | 1.1 | 9 |
| 7787 | The effect of substituents on the hydrogenation of an aldehyde catalyzed by Knöringer's catalyst. <i>Journal of Organometallic Chemistry</i> , 2014, 749, 69-74. | 0.8 | 10 |
| 7788 | The effect of C–H–O bonding and Cl– interactions in electrocatalytic dehalogenation of C2 chlorides containing an acidic hydrogen. <i>Electrochimica Acta</i> , 2014, 140, 497-504. | 2.6 | 7 |
| 7789 | Existence of a resonance hybrid structure as a result of proton tautomerism in (±)-4-Bromo-2-[(2,3-dihydroxypropylimino) methyl]phenol racemate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 120, 201-207. | 2.0 | 15 |
| 7790 | Electrochemical and spectroscopic characteristics of p-acryloyloxybenzoyl chloride and p-acryloyloxybenzoic acid and antimicrobial activity of organic compounds. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 502-513. | 2.0 | 2 |
| 7791 | Ion–ion coincidence imaging of dissociative ionization dynamics of formic acid in intense laser fields. <i>Chemical Physics</i> , 2014, 430, 40-46. | 0.9 | 9 |
| 7792 | Quantum chemical study on influence of intermolecular hydrogen bonding on the geometry, the atomic charges and the vibrational dynamics of 2,6-dichlorobenzonitrile. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 121, 464-482. | 2.0 | 35 |
| 7793 | Synthesis, characterization and quantum chemical investigation of molecular structure and vibrational spectra of 2,5-dichloro-3,6-bis-(methylamino)1,4-benzoquinone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 129, 241-254. | 2.0 | 22 |
| 7794 | Solid-state NMR strategies for the structural characterization of paramagnetic NO adducts of Frustrated Lewis Pairs (FLPs). <i>Solid State Nuclear Magnetic Resonance</i> , 2014, 61-62, 19-27. | 1.5 | 12 |
| 7795 | Theoretical study of the reaction mechanism of a series of 4-hydroxycoumarins against the DPPH radical. <i>Chemical Physics Letters</i> , 2014, 601, 116-123. | 1.2 | 7 |
| 7796 | On the formation of ethynylbiphenyl (C14D5H5; C6D5C6H4CCH) isomers in the reaction of D5-phenyl radicals (C6D5; X2A1) with phenylacetylene (C6H5C2H; X1A1) under single collision conditions. <i>Chemical Physics Letters</i> , 2014, 595-596, 230-236. | 1.2 | 13 |
| 7797 | Thermodynamic and kinetic study of ibuprofen with hydroxyl radical: A density functional theory approach. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 74-83. | 1.0 | 96 |
| 7798 | A Brief Compendium of Time-Dependent Density Functional Theory. <i>Brazilian Journal of Physics</i> , 2014, 44, 154-188. | 0.7 | 84 |
| 7799 | Selective complexation of alkali metal ions and nanotubular cyclopeptides: a DFT study. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2014, 79, 205-214. | 0.9 | 12 |
| 7800 | Redox and photoisomerisation switching the second-order nonlinear optical properties of a tetrathiafulvalene derivative across ten stable states: a DFT study. <i>Molecular Physics</i> , 2014, 112, 199-205. | 0.8 | 8 |
| 7801 | Thiadiazole derivatives as inhibitors for acidic media corrosion of artificially patinated bronze. <i>Materials and Corrosion - Werkstoffe Und Korrosion</i> , 2014, 65, 1202-1214. | 0.8 | 9 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 7802 | Electric dipole moments of the fluorescent probes Prodan and Laurdan: experimental and theoretical evaluations. <i>Biophysical Reviews</i> , 2014, 6, 63-74. | 1.5 | 24 |
| 7803 | The mechanism of the cycloaddition reaction of 1,3-dipole molecules with acetylene: an investigation with the unified reaction valley approach. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 23 |
| 7804 | Experimental and theoretical characterization of Co(III) and Zn(II) complexes with phenol-based hexa-dentate macro-acyclic ligands: synthesis, density functional theory and time-dependent density functional theory studies. <i>Journal of the Iranian Chemical Society</i> , 2014, 11, 1235-1247. | 1.2 | 2 |
| 7805 | 4-(1- <i>N</i> -amino-5-aminotetrazolyl)methylfuroxan and Its Derivatives: Synthesis, Characterization, and Energetic Properties. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 1231-1238. | 1.0 | 22 |
| 7806 | Vibrational spectra, monomer, dimer, NBO, HOMO, LUMO and NMR analyses of trans-4-hydroxy-L-proline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 54-68. | 2.0 | 8 |
| 7807 | Quest for a universal density functional: the accuracy of density functionals across a broad spectrum of databases in chemistry and physics. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2014, 372, 20120476. | 1.6 | 599 |
| 7808 | First-principle study of phase stability, electronic structure and thermodynamic properties of cadmium sulfide under high pressure. <i>Journal of Physics and Chemistry of Solids</i> , 2014, 75, 662-669. | 1.9 | 12 |
| 7809 | Update to the General Amber Force Field for Small Solutes with an Emphasis on Free Energies of Hydration. <i>Journal of Physical Chemistry B</i> , 2014, 118, 3793-3804. | 1.2 | 47 |
| 7810 | Insight into the Gas-Phase Structure of a Copper(II) <i>l</i> -Histidine Complex, the Agent Used To Treat Menkes Disease. <i>Inorganic Chemistry</i> , 2014, 53, 2349-2351. | 1.9 | 21 |
| 7811 | Copper Active Sites in Biology. <i>Chemical Reviews</i> , 2014, 114, 3659-3853. | 23.0 | 1,305 |
| 7812 | Vibrational spectra of 3,5-diamino-6-chloro-N-(diaminomethylene) pyrazine-2-carboxamide: Combined experimental and theoretical studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 127, 157-167. | 2.0 | 15 |
| 7813 | Electronic and structural properties of Au-doped zigzag boron nitride nanotubes: A DFT study. <i>Solid State Communications</i> , 2014, 189, 1-4. | 0.9 | 8 |
| 7814 | Geometrical and optical benchmarking of copper guanidine-quinoline complexes: Insights from TD-DFT and many-body perturbation theory. <i>Journal of Computational Chemistry</i> , 2014, 35, 1-17. | 1.5 | 62 |
| 7815 | The degeneracy of the Hessian eigenvalues of the $\tilde{\rho}$ -electron density: A new manifestation of aromaticity. <i>Chemical Physics Letters</i> , 2014, 595-596, 48-54. | 1.2 | 9 |
| 7816 | New dinuclear copper(I) metallacycles containing bis-Schiff base ligands fused with two 1,2,4-triazole rings: Synthesis, characterization, molecular structures and theoretical calculations. <i>Polyhedron</i> , 2014, 69, 188-196. | 1.0 | 24 |
| 7817 | How Do DFT-DCP, DFT-NL, and DFT-D3 Compare for the Description of London-Dispersion Effects in Conformers and General Thermochemistry?. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 968-980. | 2.3 | 81 |
| 7818 | A novel trigeminal zinc porphyrin and corresponding porphyrin monomers for dye-sensitized solar cells. <i>RSC Advances</i> , 2014, 4, 10439. | 1.7 | 8 |
| 7819 | Tuning the Organic Solar Cell Performance of Acceptor 2,6-Dialkylaminonaphthalene Diimides by Varying a Linker between the Imide Nitrogen and a Thiophene Group. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3433-3442. | 1.5 | 26 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7820 | Synthesis, crystal structure and properties of benzimidazole-bridged dinuclear ferrocenyl derivatives. <i>Journal of Molecular Structure</i> , 2014, 1059, 33-39. | 1.8 | 37 |
| 7822 | The reactivity game: theoretical predictions for heavy atom tunneling in adamantyl and related carbenes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 7718-7727. | 1.3 | 46 |
| 7823 | A DFT study of permanganate oxidation of toluene and its ortho-nitroderivatives. <i>Journal of Molecular Modeling</i> , 2014, 20, 2091. | 0.8 | 6 |
| 7824 | Quadruple bonding of carbon in terminal carbides. <i>Science China Chemistry</i> , 2014, 57, 426-434. | 4.2 | 14 |
| 7825 | Simulating Cl K-edge X-ray absorption spectroscopy in MCl_6^{2-} ($M = U, Np, Pu$) complexes and $UOCl_5^{-}$ using time-dependent density functional theory. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 11 |
| 7826 | Quantum chemical investigations of the water exchange mechanism on $[Al^{III}(H_2O)_5(L)]^{2+}$ as a function of the donor strength of the anionic L. <i>Journal of Molecular Modeling</i> , 2014, 20, 2083. | 0.8 | 1 |
| 7827 | Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 37 |
| 7828 | Preparation, molecular modeling and biodistribution of ^{99m}Tc -phytochlorin complex. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2014, 299, 1759-1766. | 0.7 | 9 |
| 7829 | The infrared spectra of $C_{96}H_{25}$ compared with that of $C_{96}H_{24}$. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 3 |
| 7830 | Theoretical studies of ground and excited states in a series of Zn(II) complexes, derived from thiourea and thiosemicarbazide. <i>European Physical Journal D</i> , 2014, 68, 1. | 0.6 | 2 |
| 7831 | Quantum Chemical Analysis of Uranium Trioxide Conformers. <i>Journal of Applied Spectroscopy</i> , 2014, 80, 807-812. | 0.3 | 4 |
| 7832 | QM/MM study on the catalytic mechanism of cyclohexane-1,2-dione hydrolase (CDH). <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 3 |
| 7833 | Molecular orbital closed loops analysis of the third-order NLO response of polyanion $[M_8O_{26}]^{4-}$ ($M = Cr, Mo, W$): a TDDFT study. <i>Structural Chemistry</i> , 2014, 25, 539-549. | 1.0 | 10 |
| 7834 | Synthesis, spectral and quantum chemical studies on NO-chelating sulfamonomethoxine-cyclophosph(V)azane and its Er(III) complex. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 724-729. | 2.0 | 2 |
| 7835 | Synthesis and Theoretical Investigation of a 1,8-Bis(bis(diisopropylamino)cyclopropeniminyl)naphthalene Proton Sponge Derivative. <i>Chemistry - A European Journal</i> , 2014, 20, 1032-1037. | 1.7 | 36 |
| 7836 | Phenol Quinone Tautomerism in (Arylazo)naphthols and the Analogous Schiff Bases: Benchmark Calculations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 778-789. | 1.1 | 23 |
| 7837 | Polyhydroxylated macrolide isolated from the endophytic fungus <i>Pestalotiopsis mangiferae</i> . <i>Tetrahedron Letters</i> , 2014, 55, 2642-2645. | 0.7 | 19 |
| 7838 | Quantum mechanical study of solvent effects in a prototype S_N2 reaction in solution: Cl^- attack on CH_3Cl . <i>Journal of Chemical Physics</i> , 2014, 140, 054109. | 1.2 | 16 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 7839 | Theoretical exploration on switchable NLO response induced by photochromic properties of covalently connected unsymmetrical spiropyran-polyoxometalate complex. <i>Dyes and Pigments</i> , 2014, 106, 105-110. | 2.0 | 16 |
| 7840 | Hydration properties of Cm(iii) and Th(iv) combining coordination free energy profiles with electronic structure analysis. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 5824. | 1.3 | 21 |
| 7841 | Theoretical investigation of the mechanisms of the biphenyl formation in Ni-catalyzed reductive cross-coupling system. <i>Journal of Organometallic Chemistry</i> , 2014, 757, 72-78. | 0.8 | 11 |
| 7842 | Side-Chain Engineering for Fine-Tuning of Energy Levels and Nanoscale Morphology in Polymer Solar Cells. <i>Advanced Energy Materials</i> , 2014, 4, 1400087. | 10.2 | 67 |
| 7843 | Tuning the photophysical and electrochemical properties of iridium(III) 2-aryl-1-phenylbenzimidazole complexes. <i>Inorganica Chimica Acta</i> , 2014, 415, 22-30. | 1.2 | 12 |
| 7844 | The Dark Side of Hydrogen Bonds in the Design of Optical Materials: A Charge-Density Perspective. <i>Chemistry - A European Journal</i> , 2014, 20, 2860-2865. | 1.7 | 16 |
| 7845 | Energy Decomposition Scheme Based on the Generalized Kohn-Sham Scheme. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2531-2542. | 1.1 | 130 |
| 7846 | Experimental and ab Initio Investigations of H ₂ S-Assisted Propane Oxidative Dehydrogenation Reactions. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1541-1556. | 1.1 | 11 |
| 7847 | Theoretical studies of complexes between Hg(II) ions and <i>l</i> -cysteinate amino acids. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 333-339. | 1.0 | 16 |
| 7848 | Palladium-Catalyzed <i>meta</i> -Selective C-H Bond Activation with a Nitrile-Containing Template: Computational Study on Mechanism and Origins of Selectivity. <i>Journal of the American Chemical Society</i> , 2014, 136, 344-355. | 6.6 | 317 |
| 7849 | Time-Dependent Density Functional Theory Modeling of Spin-Orbit Coupling in Ruthenium and Osmium Solar Cell Sensitizers. <i>Journal of Physical Chemistry C</i> , 2014, 118, 17067-17078. | 1.5 | 51 |
| 7850 | Photochemical Reaction Mechanism of UV-B-Induced Monomerization of UVR8 Dimers as the First Signaling Event in UV-B-Regulated Gene Expression in Plants. <i>Journal of Physical Chemistry B</i> , 2014, 118, 951-965. | 1.2 | 27 |
| 7851 | Thermodynamic and elastic properties of hexagonal ZnO under high temperature. <i>Journal of Alloys and Compounds</i> , 2014, 597, 50-57. | 2.8 | 12 |
| 7852 | The Different Inhibition Mechanisms of OXA-1 and OXA-24 β -Lactamases Are Determined by the Stability of Active Site Carboxylated Lysine. <i>Journal of Biological Chemistry</i> , 2014, 289, 6152-6164. | 1.6 | 22 |
| 7853 | Synthesis, structural, photoluminescence, vibrational and DFT investigation of the bis (4-aminopyridinium) tetrachloridocuprate(II) monohydrate. <i>Journal of Luminescence</i> , 2014, 149, 341-347. | 1.5 | 48 |
| 7854 | ESR study of spin trapping in Fenton media in the presence of taxifolin. <i>Journal of Molecular Structure</i> , 2014, 1067, 27-36. | 1.8 | 5 |
| 7855 | Blue-Violet Photoluminescence of 4-Isopropyl-pyridine Hydroxide Crystals. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3061-3067. | 1.1 | 0 |
| 7856 | Perspective: Fifty years of density-functional theory in chemical physics. <i>Journal of Chemical Physics</i> , 2014, 140, 18A301. | 1.2 | 1,083 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7857 | Mechanistic Aspects of Submolecular Copper-Catalyzed C≡N Cross-Coupling. <i>ChemCatChem</i> , 2014, 6, 1277-1282. | 1.8 | 16 |
| 7858 | Decomposition reactions of hexafluoropropylene oxide (HFPO): Rate coefficients calculated at different temperatures using ab initio and DFT reaction paths. <i>Journal of Fluorine Chemistry</i> , 2014, 159, 29-37. | 0.9 | 7 |
| 7859 | Synthetic and structural investigation of [PdBr ₂ (CNR) ₂] (R=Cy, Xyl). <i>Journal of Molecular Structure</i> , 2014, 1068, 222-227. | 1.8 | 20 |
| 7860 | Theoretical investigation on the regioselectivity of Ni(COD) ₂ -catalyzed [2+2] cycloaddition of unsymmetric diynes and CO ₂ . <i>Journal of Organometallic Chemistry</i> , 2014, 758, 45-54. | 0.8 | 11 |
| 7861 | Stereoselective Rhodium-Catalysed [2+2+2] Cycloaddition of Linear Allene-Ene/Alkene Allene Substrates: Reactivity and Theoretical Mechanistic Studies. <i>Chemistry - A European Journal</i> , 2014, 20, 5034-5045. | 1.7 | 37 |
| 7862 | Accurate Thermochemistry for Large Molecules with Modern Density Functionals. <i>Topics in Current Chemistry</i> , 2014, , 1-23. | 4.0 | 17 |
| 7863 | Molecular and electronic structure analysis of some novel copper and zinc complexes of hypervalent carbon based ligand: DFT studies. <i>Journal of Organometallic Chemistry</i> , 2014, 752, 123-132. | 0.8 | 2 |
| 7864 | Assessing electronic structure approaches for gas-ligand interactions in metal-organic frameworks: The CO ₂ -benzene complex. <i>Journal of Chemical Physics</i> , 2014, 140, 104707. | 1.2 | 20 |
| 7865 | Electronic structure of fullerene-squaraine complexes for photovoltaic devices. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 237-242. | 1.1 | 7 |
| 7866 | Redox-Controlled Hydrogen Bonding: Turning a Superbase into a Strong Hydrogen-Bond Donor. <i>Chemistry - A European Journal</i> , 2014, 20, 5914-5925. | 1.7 | 23 |
| 7867 | Magnetostructural effects of changing spin unit structure and molecular connectivity on 1H-benzimidazole functionalized radicals. <i>Polyhedron</i> , 2014, 76, 36-44. | 1.0 | 2 |
| 7868 | Capturing CO ₂ in Monoethanolamine (MEA) Aqueous Solutions: Fingerprints of Carbamate Formation Assessed with First-Principles Simulations. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1672-1677. | 2.1 | 30 |
| 7869 | Pinning the most stable H _x C _y O _z isomers in space by means of high-level theoretical procedures. <i>Chemical Physics</i> , 2014, 436-437, 22-28. | 0.9 | 43 |
| 7870 | Structural and optical properties of new cyclometalated Ru(II) derived compounds. <i>Journal of Organometallic Chemistry</i> , 2014, 760, 248-259. | 0.8 | 15 |
| 7871 | Development of Metal Cyanurates: The Example of Barium Cyanurate (BCY). <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 2536-2543. | 1.0 | 24 |
| 7872 | Capillary Atmospheric Pressure Electron Capture Ionization (cAPECI): A Highly Efficient Ionization Method for Nitroaromatic Compounds. <i>Journal of the American Society for Mass Spectrometry</i> , 2014, 25, 329-342. | 1.2 | 7 |
| 7873 | Benchmarking Hydrogen and Carbon NMR Chemical Shifts at HF, DFT, and MP2 Levels. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 572-578. | 2.3 | 152 |
| 7874 | Redox Non-Innocence of Coordinated 2-(Arylazo) Pyridines in Iridium Complexes: Characterization of Redox Series and an Insight into Voltage-Induced Current Characteristics. <i>Chemistry - A European Journal</i> , 2014, 20, 6103-6111. | 1.7 | 45 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7875 | Density functional theoretic studies of host-guest interaction in gas hydrates. Computational and Theoretical Chemistry, 2014, 1029, 26-32. | 1.1 | 24 |
| 7876 | Oxidant-Resistant Hydrogen-Bond-Donating Organocatalyst for Enantioselective Nucleophilic Epoxidation of α,β -Unsaturated Amides. Asian Journal of Organic Chemistry, 2014, 3, 403-407. | 1.3 | 20 |
| 7877 | Strengthening of hydrogen bonded coumarin 102 in ethanol solvent upon photoexcitation. New Journal of Chemistry, 2014, 38, 568-573. | 1.4 | 12 |
| 7878 | Construction of a parameter-free doubly hybrid density functional from adiabatic connection. Journal of Chemical Physics, 2014, 140, 18A512. | 1.2 | 57 |
| 7879 | Outer-valence Electron Spectra of Prototypical Aromatic Heterocycles from an Optimally Tuned Range-Separated Hybrid Functional. Journal of Chemical Theory and Computation, 2014, 10, 1934-1952. | 2.3 | 128 |
| 7880 | Flattened deltahedral structures and bridging hydrogen atoms in hypoelectronic dimolybdoxaboranes and ditungstaboranes. Journal of Organometallic Chemistry, 2014, 754, 94-103. | 0.8 | 2 |
| 7882 | Substrate-Induced Variations of Molecular Packing, Dynamics, and Intermolecular Electronic Couplings in Pentacene Monolayers on the Amorphous Silica Dielectric. ACS Nano, 2014, 8, 690-700. | 7.3 | 25 |
| 7883 | Metal-Free $C\equiv C$ Coupling Reactions with Tetraguanidino-Functionalized Pyridines and Light. Chemistry - A European Journal, 2014, 20, 5288-5297. | 1.7 | 22 |
| 7884 | On Discerning Intermolecular and Intramolecular Vibrations in Experimental Acene Spectra. Energy & Fuels, 2014, 28, 2933-2947. | 2.5 | 7 |
| 7885 | NIR Emission in Boron difluoride Complexes of 2-Hydroxychalcone Derivatives Containing an Acetonaphthone Ring. Journal of Physical Chemistry C, 2014, 118, 11906-11918. | 1.5 | 24 |
| 7886 | Ni ^I /Ru ^{II} Model for the Ni ^I State of the [NiFe]Hydrogenases: Synthesis, Spectroscopy, and Reactivity. Inorganic Chemistry, 2014, 53, 4243-4249. | 1.9 | 28 |
| 7887 | Novel D- π -A Organic Dyes with Thieno[3,2- <i>b</i>]thiophene-3,4-ethylenedioxythiophene Unit as a π -Bridge for Highly Efficient Dye-Sensitized Solar Cells with Long-Term Stability. ACS Applied Materials & Interfaces, 2014, 6, 4102-4108. | 4.0 | 48 |
| 7888 | BN-decorated graphene nanoflakes with tunable opto-electronic and charge transport properties. Journal of Materials Chemistry C, 2014, 2, 2918-2928. | 2.7 | 35 |
| 7889 | Low Symmetry Polymorph of Hydroxyapatite. Theoretical Equilibrium Morphology of the Monoclinic $Ca_5(OH)(PO_4)_3$. Crystal Growth and Design, 2014, 14, 2846-2852. | 1.4 | 26 |
| 7890 | Synthesis, spectral, theoretical studies and in vitro antimicrobial activities of novel diphenyltin(IV) complexes of Schiff bases derived from phenacylamine. Applied Organometallic Chemistry, 2014, 28, 537-544. | 1.7 | 6 |
| 7892 | Oxidative Stretching of Metal-Metal Bonds to Their Limits. Inorganic Chemistry, 2014, 53, 4777-4790. | 1.9 | 31 |
| 7893 | Determination of Size of Molecular Clusters of Ethanol by Means of NMR Diffusometry and Hydrodynamic Calculations. Journal of Physical Chemistry B, 2014, 118, 6864-6874. | 1.2 | 11 |
| 7894 | Perylene-Derived Single-Component Organic Nanoparticles with Tunable Emission: Efficient Anticancer Drug Carriers with Real-Time Monitoring of Drug Release. ACS Nano, 2014, 8, 5939-5952. | 7.3 | 102 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7895 | DFT Study on Ce-Doped Anatase TiO ₂ : Nature of Ce ³⁺ and Ti ³⁺ Centers Triggered by Oxygen Vacancy Formation. <i>Journal of Physical Chemistry C</i> , 2014, 118, 9677-9689. | 1.5 | 51 |
| 7896 | Hydration structure of Na ⁺ , K ⁺ , F ⁻ , and Cl ⁻ in ambient and supercritical water: A quantum mechanics/molecular mechanics study. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1006-1011. | 1.0 | 23 |
| 7897 | Spin-orbit interaction mediated molecular dissociation. <i>Journal of Chemical Physics</i> , 2014, 140, 184304. | 1.2 | 7 |
| 7898 | Molecular Dynamics Studies of Liposomes as Carriers for Photosensitizing Drugs: Development, Validation, and Simulations with a Coarse-Grained Model. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5-13. | 2.3 | 44 |
| 7899 | Computational study of singlet and triplet sulfonylnitrenes insertion into 1,3-butadienes: 1,2- or 1,4-cycloaddition?. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 527-531. | 0.9 | 4 |
| 7900 | On Ammonia Binding to the Oxygen-Evolving Complex of Photosystem-II: A Quantum Chemical Study. <i>Chemistry - A European Journal</i> , 2014, 20, 7300-7308. | 1.7 | 33 |
| 7901 | Switching Off the Charge Transfer and Closing the S ₁ -T ₁ ISC Channel in Excited States of Quinolizinium Derivatives: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2014, 79, 3799-3808. | 1.7 | 10 |
| 7902 | Excited state intramolecular proton transfer of 2-(2,6-dihydroxyphenyl)benzoxazole: Insights using computational methods. <i>Journal of Luminescence</i> , 2014, 154, 267-273. | 1.5 | 9 |
| 7903 | Synthesis, crystal structure and photochromism of new diarylethenes with a benzene moiety. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 131, 235-242. | 2.0 | 6 |
| 7904 | Triple associates based on (oxime)Pt(II) species, 18-crown-6, and water: Synthesis, structural characterization, and DFT study. <i>Journal of Molecular Structure</i> , 2014, 1068, 176-181. | 1.8 | 5 |
| 7905 | Sulfur X-ray absorption fine structure in porous Li-S cathode films measured under argon atmospheric conditions. <i>Spectrochimica Acta, Part B: Atomic Spectroscopy</i> , 2014, 94-95, 22-26. | 1.5 | 6 |
| 7906 | Thermochemistry of 1,1,3,3-tetramethylguanidine and 1,1,3,3-tetramethylguanidinium nitrate. <i>Journal of Chemical Thermodynamics</i> , 2014, 77, 179-189. | 1.0 | 17 |
| 7907 | Vibrations and reorientations of H ₂ O molecules in [Sr(H ₂ O) ₆]Cl ₂ studied by Raman light scattering, incoherent inelastic neutron scattering and proton magnetic resonance. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 124, 429-440. | 2.0 | 9 |
| 7908 | Facts, Presumptions, and Myths on the Solvent-Free and Catalyst-Free Biginelli Reaction. What is Catalysis for?. <i>Journal of Organic Chemistry</i> , 2014, 79, 3383-3397. | 1.7 | 82 |
| 7909 | Analysis of the Configurations of a Crystal Surface. Pyrope (Mg ₃ Al ₂ Si ₃ O ₁₂) as a Case Study. <i>Crystal Growth and Design</i> , 2014, 14, 2357-2365. | 1.4 | 7 |
| 7910 | Theoretical Study of POCOP-Pincer Iridium(III)/Iron(II) Hydride Catalyzed Hydrosilylation of Carbonyl Compounds: Hydride Not Involved in the Iridium(III) System but Involved in the Iron(II) System. <i>Organometallics</i> , 2014, 33, 847-857. | 1.1 | 43 |
| 7911 | Sensitivity of ab Initio vs Empirical Methods in Computing Structural Effects on NMR Chemical Shifts for the Example of Peptides. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 122-133. | 2.3 | 20 |
| 7912 | DFT study on the organocatalytic carbonyl-olefin metathesis. <i>Computational and Theoretical Chemistry</i> , 2014, 1027, 179-185. | 1.1 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 7913 | Density Functional Theory of Open-Shell Systems. The 3d-Series Transition-Metal Atoms and Their Cations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 102-121. | 2.3 | 65 |
| 7914 | Theoretical studies on the structures and electronic spectra of carbon chains C _n N (n=3-12). <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 2 |
| 7915 | On the Innocence of Bipyridine Ligands: How Well Do DFT Functionals Fare for These Challenging Spin Systems?. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 220-235. | 2.3 | 34 |
| 7916 | Kinetic studies of hydroxyquinone formation from water soluble benzoquinones. <i>New Journal of Chemistry</i> , 2014, 38, 588-597. | 1.4 | 8 |
| 7917 | Blue phosphorescent nitrile containing C [*] cyclometalated NHC platinum complexes. <i>Dalton Transactions</i> , 2014, 43, 3297-3305. | 1.6 | 46 |
| 7918 | New Approach to Tolman's Electronic Parameter Based on Local Vibrational Modes. <i>Inorganic Chemistry</i> , 2014, 53, 478-495. | 1.9 | 61 |
| 7919 | Theoretical Study of Novel Azo-Tetraphenylporphyrins: Potential Photovoltaic Materials. <i>Journal of Physical Chemistry A</i> , 2014, 118, 197-207. | 1.1 | 5 |
| 7920 | Interaction between O ₂ and neutral/charged Au (n= 1-3) clusters: A comparative study between density-functional theory and coupled cluster calculations. <i>Chemical Physics Letters</i> , 2014, 592, 127-131. | 1.2 | 15 |
| 7921 | Agostic Interactions in Nickel(II) Complexes: Trans Influence of Ancillary Ligands on the Strength of the Bond. <i>Organometallics</i> , 2014, 33, 84-93. | 1.1 | 21 |
| 7922 | A comparative study of polymers containing naphthodifuranone and benzodifuranone units in the main chain. <i>Polymer Chemistry</i> , 2014, 5, 646-652. | 1.9 | 13 |
| 7923 | 25th Anniversary Article: Design of Polymethine Dyes for All-Optical Switching Applications: Guidance from Theoretical and Computational Studies. <i>Advanced Materials</i> , 2014, 26, 68-84. | 11.1 | 97 |
| 7924 | Deltahedral ferratricarbaboranes: analogues of ferrocene. <i>Dalton Transactions</i> , 2014, 43, 4993-5000. | 1.6 | 9 |
| 7925 | Spectral and quantum chemical studies on 1,3-bis(N1-4-amino-6-methoxypyrimidinebenzenesulfonamide-2,2,4,4-ethane-1,2-dithiol)-2,4-dichlorocyclodiphosph(V)azane and its erbium complex. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 118, 481-487. | 2.0 | 1 |
| 7926 | Dicobalt- μ_4 -oxo Polyoxometalate Compound, [(μ_2 -P ₂ W ₁₇ O ₆₁ Co) ₂ O] ¹⁴⁻ : A Potent Species for Water Oxidation, C-H Bond Activation, and Oxygen Transfer. <i>Inorganic Chemistry</i> , 2014, 53, 1779-1787. | 1.9 | 30 |
| 7927 | Electron delocalization index based on bond order orbitals. <i>Chemical Physics Letters</i> , 2014, 593, 154-159. | 1.2 | 37 |
| 7928 | Influence of the Coordination Environment of Zinc(II) Complexes of Designed Mannich Ligands on Phosphatase Activity: A Combined Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , 2014, 53, 85-96. | 1.9 | 72 |
| 7929 | Theoretical investigations on the molecular structure, vibrational spectra, thermodynamics, HOMO-LUMO, NBO analyses and paramagnetic susceptibility properties of p-(p-hydroxyphenoxy)benzoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 121, 575-585. | 2.0 | 17 |
| 7930 | Experimental and Theoretical Study on Palladium-Catalyzed C-P Bond Formation via Direct Coupling of Triarylbiaryls with P(O)H Compounds. <i>Journal of Organic Chemistry</i> , 2014, 79, 608-617. | 1.7 | 76 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7931 | Computations Offer an Unconventional Route to Metallaphosphabenzene from a Half-Phosphametalloocene. <i>Organometallics</i> , 2014, 33, 817-822. | 1.1 | 26 |
| 7932 | Breaking conjugation: unusual regioselectivity with 2-substituted allylic substrates in the Tsuji-Trost reaction. <i>Chemical Science</i> , 2014, 5, 1241-1250. | 3.7 | 9 |
| 7933 | Theoretical investigations on the reaction kinetics of CH ₃ OCl/CD ₃ OCl with chloride ion. <i>Computational and Theoretical Chemistry</i> , 2014, 1031, 69-75. | 1.1 | 3 |
| 7934 | Unexpectedly High Barriers to M ⁺ P Rotation in Tertiary Phobane Complexes: PhobPR Behavior That Is Commensurate with tBu ₂ PR. <i>Organometallics</i> , 2014, 33, 702-714. | 1.1 | 3 |
| 7935 | Origins of Selective C(sp ²)-H Activation Using Transition Metal Complexes with N,N-Bidentate Directing Groups: A Combined Theoretical-Experimental Study. <i>ACS Catalysis</i> , 2014, 4, 649-656. | 5.5 | 51 |
| 7936 | Classical simulation of acid and base dissociation constants in supercritical water at constant density. <i>Journal of Supercritical Fluids</i> , 2014, 86, 145-149. | 1.6 | 2 |
| 7937 | Engineering Frontier Energy Levels in Donor-Acceptor Fluoren-9-ylidene Malononitriles versus Fluorenones. <i>Journal of Physical Chemistry A</i> , 2014, 118, 475-486. | 1.1 | 22 |
| 7938 | Uquantchem: A versatile and easy to use quantum chemistry computational software. <i>Computer Physics Communications</i> , 2014, 185, 415-421. | 3.0 | 5 |
| 7939 | Terpyridine-Triarylborane Conjugates for the Dual Complexation of Zinc(II) Cation and Fluoride Anion. <i>Organometallics</i> , 2014, 33, 753-762. | 1.1 | 35 |
| 7940 | Biosynthetic consequences of multiple sequential post-transition-state bifurcations. <i>Nature Chemistry</i> , 2014, 6, 104-111. | 6.6 | 128 |
| 7941 | Structures and bonding characters of (MgO) _{3n} (n = 2-8) clusters. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2014, 47, 025102. | 0.6 | 19 |
| 7942 | Exploring CO dissociation on Fe nanoparticles by density functional theory-based methods: Fe ₁₃ as a case study. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 7 |
| 7944 | Dye chemistry with time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14334-14356. | 1.3 | 294 |
| 7945 | Computational modeling of single- versus double-anchoring modes in di-branched organic sensitizers on TiO ₂ surfaces: structural and electronic properties. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4709-4719. | 1.3 | 28 |
| 7946 | Biomolecular Mode of Action of Metformin in Relation to Its Copper Binding Properties. <i>Biochemistry</i> , 2014, 53, 787-795. | 1.2 | 46 |
| 7947 | Analysis of Seven-Membered Lactones by Computational NMR Methods: Proton NMR Chemical Shift Data are More Discriminating than Carbon. <i>Journal of Organic Chemistry</i> , 2014, 79, 752-758. | 1.7 | 39 |
| 7948 | Theoretical and Experimental Vibrational Spectroscopic Investigation of Two R ₁ R ₂ -Diphenylsilyl-Containing Monomers and Their Optically Active Derivative Polymer. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1175-1184. | 1.1 | 8 |
| 7949 | Description of Aromaticity with the Help of Vibrational Spectroscopy: Anthracene and Phenanthrene. <i>Journal of Physical Chemistry A</i> , 2014, 118, 223-237. | 1.1 | 67 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7950 | Toward an Accurate Description of Methane Physisorption on Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2014, 118, 544-550. | 1.5 | 22 |
| 7951 | Conformational Equilibria in Butane-1,4-diol: A Benchmark of a Prototypical System with Strong Intramolecular H-bonds. <i>Journal of Physical Chemistry A</i> , 2014, 118, 293-303. | 1.1 | 53 |
| 7952 | On-Water Reactivity and Regioselectivity of Quinones in C–N Coupling with Amines: Experimental and Theoretical Study. <i>Australian Journal of Chemistry</i> , 2014, 67, 217. | 0.5 | 6 |
| 7953 | Impact of Spin–Orbit Coupling on Photocurrent Generation in Ruthenium Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 375-380. | 2.1 | 31 |
| 7954 | Peculiar structure of the potential energy surfaces of typical electrocyclic reactions in the areas of the symmetry-forbidden reaction paths. <i>Computational and Theoretical Chemistry</i> , 2014, 1030, 44-52. | 1.1 | 5 |
| 7955 | 2,3-Dihydroimidazo[1,2-b]ferroceno[d]pyridazines and a 3,4-dihydro-2H-pyrimido[1,2-b]ferroceno[d]pyridazine: Synthesis, structure and in vitro antiproliferation activity on selected human cancer cell lines. <i>Journal of Organometallic Chemistry</i> , 2014, 750, 41-48. | 0.8 | 17 |
| 7956 | The impact of surface structure and band gap on the optoelectronic properties of Cu ₂ O nanoclusters of varying size and symmetry. <i>RSC Advances</i> , 2014, 4, 5092. | 1.7 | 23 |
| 7957 | Novel triphenylamine-modified ruthenium(ii) terpyridine complexes for nickel oxide-based cathodic dye-sensitized solar cells. <i>RSC Advances</i> , 2014, 4, 5782. | 1.7 | 37 |
| 7958 | Solvatochromic Fluorescent 2-Substituted 3-Ethynyl Quinoxalines: Four-Component Synthesis, Photophysical Properties, and Electronic Structure. <i>Journal of Organic Chemistry</i> , 2014, 79, 3296-3310. | 1.7 | 70 |
| 7959 | A green catalysis of CO ₂ fixation to aliphatic cyclic carbonates by a new ionic liquid system. <i>Applied Catalysis A: General</i> , 2014, 472, 160-166. | 2.2 | 34 |
| 7960 | Monoisomeric Phthalocyanines and Phthalocyanine–Fullerene Dyads with Polar Side Chains: Synthesis, Modeling, and Photovoltage. <i>Journal of Physical Chemistry C</i> , 2014, 118, 2754-2765. | 1.5 | 12 |
| 7961 | 1,3,2-Dioxaphospholanes with an Annelated 1,2-Dicarba-dodecaborane(12) Unit: Formation and Dimerization. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 233-246. | 1.0 | 9 |
| 7962 | A New-Generation Density Functional. <i>Springer Briefs in Molecular Science</i> , 2014, , . | 0.1 | 20 |
| 7963 | Selective synthesis of indazoles and indoles via triazene–alkyne cyclization switched by different metals. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 1061-1071. | 1.5 | 25 |
| 7964 | Capricious Selectivity in Electrophilic Deuteration of Methylendioxy Substituted Aromatic Compounds. <i>Journal of Organic Chemistry</i> , 2014, 79, 10636-10640. | 1.7 | 12 |
| 7965 | Theoretical investigation of the effect of the solvent, hydrogen bond and amino group on the isomerization of Rhodamines. <i>Computational and Theoretical Chemistry</i> , 2014, 1050, 1-6. | 1.1 | 10 |
| 7966 | Photocatalytic reactions of a nickel(II) annulene complex incorporated in polymeric structures. <i>RSC Advances</i> , 2014, 4, 53157-53171. | 1.7 | 3 |
| 7967 | Role of the Base in Buchwald–Hartwig Amination. <i>Journal of Organic Chemistry</i> , 2014, 79, 11961-11969. | 1.7 | 74 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 7968 | Turn-on Phosphorescent Chemodosimeter for Hg ²⁺ Based on a Cyclometalated Ir(III) Complex and Its Application in Time-Resolved Luminescence Assays and Live Cell Imaging. <i>Inorganic Chemistry</i> , 2014, 53, 11498-11506. | 1.9 | 51 |
| 7969 | Electrochemical oxidation of imazapyr with BDD electrode in titanium substrate. <i>Chemosphere</i> , 2014, 117, 596-603. | 4.2 | 27 |
| 7970 | Biologically inspired pteridine redox centres for rechargeable batteries. <i>Nature Communications</i> , 2014, 5, 5335. | 5.8 | 254 |
| 7971 | Computational Chemistry Meets Experiments for Explaining the Behavior of Bibenzyl: A Thermochemical and Spectroscopic (Infrared, Raman, and NMR) Investigation. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5586-5592. | 2.3 | 22 |
| 7972 | Axial Chirality of 4-Arylpyrazolo[3,4- <i>b</i>]pyridines. Conformational Analysis and Absolute Configuration. <i>Journal of Organic Chemistry</i> , 2014, 79, 11039-11050. | 1.7 | 25 |
| 7973 | One-versus Two-Electron Oxidation of Complexed Guanidino-Functionalized Aromatic Compounds. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 6039-6050. | 1.0 | 26 |
| 7974 | Enthalpy of Formation of Anisole: Implications for the Controversy on the O-H Bond Dissociation Enthalpy in Phenol. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11026-11032. | 1.1 | 28 |
| 7975 | Homologation of Boronic Esters with Organolithium Compounds: A Computational Assessment of Mechanism. <i>Journal of Organic Chemistry</i> , 2014, 79, 12148-12158. | 1.7 | 30 |
| 7976 | Energy States of Ligand Capped Ag Nanoparticles: Relating Surface Plasmon Resonance to Work Function. <i>Journal of Physical Chemistry C</i> , 2014, 118, 24827-24832. | 1.5 | 15 |
| 7977 | Monitoring of Reaction Intermediates in the Gas Phase: Ruthenium-Catalyzed C-C Coupling. <i>Organometallics</i> , 2014, 33, 6868-6878. | 1.1 | 22 |
| 7978 | The mechanism of transition-metal (Cu or Pd)-catalyzed synthesis of benzimidazoles from amidines: theoretical investigation. <i>Dalton Transactions</i> , 2014, 43, 16769-16779. | 1.6 | 9 |
| 7979 | Assessment of Franck-Condon Methods for Computing Vibrationally Broadened UV-vis Absorption Spectra of Flavin Derivatives: Riboflavin, Roseoflavin, and 5-Thioflavin. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5549-5566. | 2.3 | 44 |
| 7980 | Vibronic-structure tracking: A shortcut for vibrationally resolved UV/Vis-spectra calculations. <i>Journal of Chemical Physics</i> , 2014, 141, 164115. | 1.2 | 13 |
| 7981 | Viability of Nonclassical Carbocations Proposed as Intermediates in the Biosynthesis of Atiserene, Beyerene, Kaurene, and Trachylobane Diterpenes. <i>Helvetica Chimica Acta</i> , 2014, 97, 1475-1480. | 1.0 | 6 |
| 7982 | Insights into the influence of dispersion correction in the theoretical treatment of guanidine-quinoline copper(I) complexes. <i>Journal of Computational Chemistry</i> , 2014, 35, 1943-1950. | 1.5 | 55 |
| 7983 | Spin-orbit effects in square-planar Pt(σ) complexes with bidentate and terdentate ligands: theoretical absorption/emission spectroscopy. <i>Dalton Transactions</i> , 2014, 43, 17806-17819. | 1.6 | 41 |
| 7984 | The MC-DFT approach including the SCS-MP2 energies to the new minnesota-type functionals. <i>Journal of Computational Chemistry</i> , 2014, 35, 1560-1567. | 1.5 | 4 |
| 7985 | Why Does the Coordination Mode of Physiological Bis(σ -L)histidinato)copper(II) Differ in the Gas Phase, Crystal Lattice, and Aqueous Solutions? A Quantum Chemical Study. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 198-212. | 1.0 | 6 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 7986 | Six-Vertex Hydrogen-Rich Cp ₂ M ₂ B ₄ H ₈ Dimetallaboranes of the Second- and Third-Row Transition Metals: Effects of Skeletal Electron Count on Preferred Polyhedra. <i>Organometallics</i> , 2014, 33, 6443-6451. | 1.1 | 7 |
| 7987 | On the full exploitation of symmetry in periodic (as well as molecular) self-consistent-field <i>ab initio</i> calculations. <i>Journal of Chemical Physics</i> , 2014, 141, 104108. | 1.2 | 21 |
| 7988 | Exploitation of symmetry in periodic Self-Consistent-Field <i>ab initio</i> calculations: application to large three-dimensional compounds. <i>Science China Chemistry</i> , 2014, 57, 1418-1426. | 4.2 | 4 |
| 7989 | Electronic Structure of the Positive Radical of ¹³ C-Labeled Poly(3-Octylthienylene Vinylene) Polymer. <i>Applied Magnetic Resonance</i> , 2014, 45, 827-839. | 0.6 | 2 |
| 7990 | Gas-Phase Valence-Electron Photoemission Spectroscopy Using Density Functional Theory. <i>Topics in Current Chemistry</i> , 2014, 347, 137-191. | 4.0 | 37 |
| 7991 | Impact of Ground- and Excited-State Aromaticity on Cyclopentadiene and Silole Excitation Energies and Excited-State Polarities. <i>Chemistry - A European Journal</i> , 2014, 20, 9295-9303. | 1.7 | 61 |
| 7992 | Status in Calculating Electronic Excited States in Transition Metal Oxides from First Principles. <i>Topics in Current Chemistry</i> , 2014, 347, 47-98. | 4.0 | 15 |
| 7993 | Competition between photodetachment and autodetachment of the $m\{2^1\pi\pi^*\}$ state of the green fluorescent protein chromophore anion. <i>Journal of Chemical Physics</i> , 2014, 140, 205103. | 1.2 | 21 |
| 7994 | Water on BN doped benzene: A hard test for exchange-correlation functionals and the impact of exact exchange on weak binding. <i>Journal of Chemical Physics</i> , 2014, 141, 18C530. | 1.2 | 25 |
| 7995 | Computational Reference Data for the Photochemistry of Cyclobutane Pyrimidine Dimers. <i>ChemPhysChem</i> , 2014, 15, 3342-3354. | 1.0 | 20 |
| 7996 | Description of electron transfer in the ground and excited states of organic donor-acceptor systems by single-reference and multi-reference density functional methods. <i>Journal of Chemical Physics</i> , 2014, 141, 124123. | 1.2 | 14 |
| 7997 | Impact of Electron Delocalization on the Nature of the Charge-Transfer States in Model Pentacene/C ₆₀ Interfaces: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 27648-27656. | 1.5 | 80 |
| 7998 | Facile Smiles-type rearrangement in radical cations of <i>N</i> -acyl arylsulfonamides and analogs. <i>Rapid Communications in Mass Spectrometry</i> , 2014, 28, 829-834. | 0.7 | 8 |
| 7999 | Understanding the Guanidine-Like Cationic Moiety for Optimal Binding into the DNA Minor Groove. <i>ChemMedChem</i> , 2014, 9, 2065-2073. | 1.6 | 15 |
| 8000 | Ligand-Centered Redox in Nickel(II) Complexes of 2-(Arylazo)pyridine and Isolation of 2-Pyridyl-Substituted Triaryl Hydrazines via Catalytic <i>N</i> -Arylation of Azo-Function. <i>Inorganic Chemistry</i> , 2014, 53, 12002-12013. | 1.9 | 33 |
| 8001 | Computational Mechanistic Study of Fe-Catalyzed Hydrogenation of Esters to Alcohols: Improving Catalysis by Accelerating Precatalyst Activation with a Lewis Base. <i>ACS Catalysis</i> , 2014, 4, 4377-4388. | 5.5 | 91 |
| 8002 | Unraveling the Mechanism of a Reversible Photoactivated Molecular Proton Crane. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12965-12971. | 1.2 | 20 |
| 8003 | In Situ XAFS and HAXPES Analysis and Theoretical Study of Cobalt Polypyrrole Incorporated on Carbon (CoPPyC) Oxygen Reduction Reaction Catalysts for Anion-Exchange Membrane Fuel Cells. <i>Journal of Physical Chemistry C</i> , 2014, 118, 25480-25486. | 1.5 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8004 | Four-Component Fluorescence of <i>trans</i> -1,2-Di(1-methyl-2-naphthyl)ethene at 77 K in Glassy Media. Conformational Subtleties Revealed. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10575-10586. | 1.1 | 8 |
| 8005 | C ⁺ Hydrogen Atom Transfer in Post-Cleavage Radical-Cation Complexes: Short and Steep versus Long Winding Road. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10797-10803. | 1.1 | 6 |
| 8006 | Alcohol oxidation reactions catalyzed by ruthenium ^{II} carbonyl complexes of thioaryloimidazoles. <i>Applied Organometallic Chemistry</i> , 2014, 28, 641-651. | 1.7 | 23 |
| 8007 | Interaction Energy of Large Molecules from Restrained Denominator MP2-F12. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4857-4861. | 2.3 | 12 |
| 8008 | Kinetic model and mechanism of the acid dissociation of d-metal bis(dipyrrolylmethenates). <i>Kinetics and Catalysis</i> , 2014, 55, 391-400. | 0.3 | 2 |
| 8009 | Reactions of dichlorocarbene, dichlorosilylene, and dichlorogermylene with carboranes(12). A theoretical study. <i>Russian Journal of General Chemistry</i> , 2014, 84, 1330-1338. | 0.3 | 3 |
| 8010 | Role of Proton Hopping in Surface Charge Transport on Tin Dioxide As Revealed by the Thermal Dependence of Conductance. <i>Journal of Physical Chemistry A</i> , 2014, 118, 12031-12040. | 1.1 | 10 |
| 8011 | Time-dependent approach to spin-vibronic coupling: Implementation and assessment. <i>Journal of Chemical Physics</i> , 2014, 140, 114104. | 1.2 | 81 |
| 8012 | Substituent effects on fluorescence properties of thiazolo[4,5-b]pyrazine derivatives. <i>Photochemical and Photobiological Sciences</i> , 2014, 13, 1765-1772. | 1.6 | 8 |
| 8013 | On the thermal Pummerer rearrangement of substituted sulfoxides. <i>Journal of Sulfur Chemistry</i> , 2014, 35, 248-260. | 1.0 | 0 |
| 8014 | Understanding excitation energy transfer in metalloporphyrin heterodimers with different linkers, bonding structures, and geometries through stimulated X-ray Raman spectroscopy. <i>Journal of Modern Optics</i> , 2014, 61, 558-567. | 0.6 | 8 |
| 8015 | The applicability of proton transfer reaction-mass spectrometry (PTR-MS) for determination of isocyanic acid (ICA) in work room atmospheres. <i>Environmental Sciences: Processes and Impacts</i> , 2014, 16, 2423-2431. | 1.7 | 16 |
| 8016 | A hybrid bis(amino-styryl) substituted Bodipy dye and its conjugate diacid: synthesis, structure, spectroscopy and quantum chemical calculations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10187. | 1.3 | 25 |
| 8017 | An isomeric reaction benchmark set to test if the performance of state-of-the-art density functionals can be regarded as independent of the external potential. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14559. | 1.3 | 15 |
| 8018 | A detailed investigation of light-harvesting efficiency of blue color emitting divergent iridium dendrimers with peripheral phenylcarbazole units. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4510-4521. | 1.3 | 26 |
| 8019 | Ab initio calculations on the ¹ O ₂ quenching mechanism by trans-resveratrol. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 12773-12781. | 1.3 | 16 |
| 8020 | A DFT study of the mechanism of copper-catalyzed synthesis of 2H-indazoles from aryl azide. <i>Dalton Transactions</i> , 2014, 43, 55-62. | 1.6 | 5 |
| 8021 | Double exchange in a mixed-valent octanuclear iron cluster, [Fe ₈ (¹ / ₄ -O) ₄ (¹ / ₄ -4-Cl-pz) ₁₂ Cl ₄] ¹⁶⁺ . <i>Dalton Transactions</i> , 2014, 43, 11269-11276. | 1.6 | 11 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8022 | Receding mechanism of NLO response of polyanion $[M_8O_{26}]^{4-}$ (M = Cr, Mo, W) and the closed loops theory analysis. <i>New Journal of Chemistry</i> , 2014, 38, 2619-2628. | 1.4 | 3 |
| 8023 | Enhancement of nonlinear optical properties in late group 15 tetrasubstituted cubanes. <i>Dalton Transactions</i> , 2014, 43, 6333-6338. | 1.6 | 1 |
| 8024 | Flexible bonding between copper and nitric oxide: infrared photodissociation spectroscopy of copper nitrosyl cation complexes: $[Cu(NO)_n]^+$ (n = 1-5). <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10788. | 1.3 | 14 |
| 8025 | Raman Spectroscopy of Conformational Rearrangements at Low Temperatures. <i>Springer Theses</i> , 2014, , . | 0.0 | 4 |
| 8026 | Unbranched n-Alkanes. <i>Springer Theses</i> , 2014, , 37-117. | 0.0 | 2 |
| 8027 | Theoretical Study of Solvent Effects on the Ground and Low-Lying Excited Free Energy Surfaces of a Push-Pull Substituted Azobenzene. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12518-12530. | 1.2 | 18 |
| 8028 | Comparing random and regular diketopyrrolopyrrole-bithiophene-thienopyrrolodione terpolymers for organic photovoltaics. <i>Journal of Materials Chemistry A</i> , 2014, 2, 17899-17905. | 5.2 | 76 |
| 8029 | Inaccessibility of the $\frac{1}{4}$ -hydride species in $[FeFe]$ hydrogenases. <i>Chemical Science</i> , 2014, 5, 215-221. | 3.7 | 48 |
| 8030 | Photoreduction and light-induced triplet-state formation in a single-site fluoroalkylated zinc phthalocyanine. <i>Dalton Transactions</i> , 2014, 43, 14942-14948. | 1.6 | 13 |
| 8031 | A QM/MM MD study of the pH-dependent ring-opening catalysis and lid motif flexibility in glucosamine 6-phosphate deaminase. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18406-18417. | 1.3 | 12 |
| 8032 | Chemiluminescent 2,6-diphenylimidazo[1,2-a]pyrazin-3(7H)-ones: a new entry to Cypridina luciferin analogues. <i>Photochemical and Photobiological Sciences</i> , 2014, 13, 182-189. | 1.6 | 10 |
| 8033 | Unimolecular reaction chemistry of a charge-tagged beta-hydroxyperoxyl radical. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24954-24964. | 1.3 | 9 |
| 8034 | Charting the mechanism and reactivity of zirconium oxalate with hydroxamate ligands using density functional theory: implications in new chelate design. <i>Dalton Transactions</i> , 2014, 43, 9872-9884. | 1.6 | 44 |
| 8035 | Modeling of photoactive conjugated donor-acceptor copolymers: the effect of the exact HF exchange in DFT functionals on geometries and gap energies of oligomer and periodic models. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 13294-13305. | 1.3 | 29 |
| 8036 | The reasons for ligand-dependent quantum yields and spectroscopic properties of platinum complexes based on tetradentate $O^{\wedge}N^{\wedge}C^{\wedge}N$ ligands: a DFT and TD-DFT study. <i>Dalton Transactions</i> , 2014, 43, 2849-2858. | 1.6 | 7 |
| 8037 | Probing the metallating ability of a polybasic sodium alkylmagnesiato supported by a bulky bis(amido) ligand: deprotomagnesiato reactions of nitrogen-based aromatic substrates. <i>Dalton Transactions</i> , 2014, 43, 4361-4369. | 1.6 | 14 |
| 8038 | A density functional study of the spin state energetics of polypyrazolylborato complexes of first-row transition metals. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14514. | 1.3 | 20 |
| 8039 | Ultrafast resonance energy transfer in the umbelliferone-alizarin bichromophore. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10059-10074. | 1.3 | 12 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 8040 | Quantum-chemical insights into mixed-valence systems: within and beyond the Robin-Day scheme. <i>Chemical Society Reviews</i> , 2014, 43, 5067-5088. | 18.7 | 168 |
| 8041 | A density functional theory study of the mechanism of isomerization of 2-aryl-2H-azirines to 2,3-disubstituted indoles by FeCl ₂ and Rh ₂ (O ₂ CCF ₃) ₄ . <i>Dalton Transactions</i> , 2014, 43, 5364. | 1.6 | 9 |
| 8042 | Investigation of ternary ConCN ⁿ /O (n = 1-5) clusters by density functional calculations. <i>Dalton Transactions</i> , 2014, 43, 5516. | 1.6 | 9 |
| 8043 | Pentalene formation mechanisms redux. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 887-894. | 1.5 | 24 |
| 8044 | Photophysics of Flavin Derivatives Absorbing in the Blue-Green Region: Thioflavins As Potential Cofactors of Photoswitches. <i>Journal of Physical Chemistry B</i> , 2014, 118, 1743-1753. | 1.2 | 18 |
| 8045 | Evaluation of CM5 Charges for Condensed-Phase Modeling. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2802-2812. | 2.3 | 54 |
| 8046 | Breaking Down the Reactivity of λ^3 -Iodanes: The Impact of Structure and Bonding on Competing Reaction Mechanisms. <i>Journal of Organic Chemistry</i> , 2014, 79, 8374-8382. | 1.7 | 19 |
| 8047 | Femtosecond Laser Spectroscopy and DFT Studies of Photochromic Dithizonatomercury Complexes. <i>Journal of Physical Chemistry A</i> , 2014, 118, 844-855. | 1.1 | 10 |
| 8048 | Torque-selective Ring Opening of Fused Cyclobutenamides: Evidence for a <i>cis,trans</i> -Cyclooctadienone Intermediate. <i>Journal of the American Chemical Society</i> , 2014, 136, 9802-9805. | 6.6 | 27 |
| 8049 | Revisiting the role of exact exchange in DFT spin-state energetics of transition metal complexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14479-14488. | 1.3 | 68 |
| 8050 | Optical excitation of MgO nanoparticles; a computational perspective. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22052-22061. | 1.3 | 33 |
| 8051 | How Cinchona Alkaloid-Derived Primary Amines Control Asymmetric Electrophilic Fluorination of Cyclic Ketones. <i>Journal of the American Chemical Society</i> , 2014, 136, 9556-9559. | 6.6 | 64 |
| 8052 | Probing the Role of Secondary versus Tertiary Amine Donor Ligands for Indium Catalysts in Lactide Polymerization. <i>Inorganic Chemistry</i> , 2014, 53, 9897-9906. | 1.9 | 35 |
| 8053 | Chemistry of Diruthenium Analogue of Pentaborane(9) With Heterocumulenes: Toward Novel Trimetallic Cubane-Type Clusters. <i>Inorganic Chemistry</i> , 2014, 53, 10527-10535. | 1.9 | 52 |
| 8054 | Antibacterial drugs as corrosion inhibitors for bronze surfaces in acidic solutions. <i>Applied Surface Science</i> , 2014, 321, 188-196. | 3.1 | 51 |
| 8055 | Optical rotation calculations on large molecules using the approximate coupled cluster model CC2 and the resolution-of-the-identity approximation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 5942. | 1.3 | 14 |
| 8056 | The nuclear electric quadrupole moment of copper. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 11590-11596. | 1.3 | 11 |
| 8057 | Biomolecular structure manipulation using tailored electromagnetic radiation: a proof of concept on a simplified model of the active site of bacterial DNA topoisomerase. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21768-21777. | 1.3 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 8058 | Polymeric watersplitting photocatalysts; a computational perspective on the water oxidation conundrum. <i>Journal of Materials Chemistry A</i> , 2014, 2, 11996-12004. | 5.2 | 55 |
| 8059 | The substituent effect on benzene dications. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4752-4763. | 1.3 | 17 |
| 8060 | Synthesis, characterization and crystal structure analysis of cobaltaborane and cobaltaheteroborane clusters. <i>Dalton Transactions</i> , 2014, 43, 9976-9985. | 1.6 | 22 |
| 8061 | Computational study of the working mechanism and rate acceleration of overcrowded alkene-based light-driven rotary molecular motors. <i>RSC Advances</i> , 2014, 4, 10240. | 1.7 | 21 |
| 8062 | Structural modification strategies for the rational design of red/NIR region BODIPYs. <i>Chemical Society Reviews</i> , 2014, 43, 4778-4823. | 18.7 | 1,076 |
| 8063 | Experimental and theoretical studies on the mechanism for chemical oxidation of multiwalled carbon nanotubes. <i>RSC Advances</i> , 2014, 4, 28826-28831. | 1.7 | 31 |
| 8064 | Large-scale virtual high-throughput screening for the identification of new battery electrolyte solvents: evaluation of electronic structure theory methods. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 7919-7926. | 1.3 | 81 |
| 8065 | DFT studies on the mechanism of palladium-catalyzed carbon-silicon cleavage for the synthesis of benzosilole derivatives. <i>Dalton Transactions</i> , 2014, 43, 11138-11144. | 1.6 | 22 |
| 8066 | Photocrystallographic Observation of Halide-Bridged Intermediates in Halogen Photoeliminations. <i>Journal of the American Chemical Society</i> , 2014, 136, 15346-15355. | 6.6 | 31 |
| 8067 | Description of heteroaromaticity on the basis of π -electron density anisotropy. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 11538. | 1.3 | 15 |
| 8068 | Halogen-halogen interactions and halogen bonding in thiacalixarene systems. <i>CrystEngComm</i> , 2014, 16, 2605-2614. | 1.3 | 26 |
| 8069 | Formation and Stability of C_6H_3 Isomers. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10109-10116. | 1.1 | 8 |
| 8070 | Effects of resonant excitation, pulse duration and intensity on photoelectron imaging of a dianion. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 489-496. | 1.3 | 11 |
| 8071 | Theoretical study on the stability of osmasilabenzynes. <i>Dalton Transactions</i> , 2014, 43, 7570. | 1.6 | 23 |
| 8072 | The derivative discontinuity of the exchange-correlation functional. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14378-14387. | 1.3 | 74 |
| 8073 | An enantioselective Diels-Alder reaction of 1,2-dihydropyridines with α -acyloxyacroleins catalyzed by a chiral primary ammonium salt. <i>Chemical Communications</i> , 2014, 50, 6357-6360. | 2.2 | 21 |
| 8074 | Coordination and conformational isomers in mononuclear iron complexes with pertinence to the [FeFe] hydrogenase active site. <i>Dalton Transactions</i> , 2014, 43, 4537-4549. | 1.6 | 43 |
| 8075 | Rationalizing the Lacking of Inversion Symmetry in a Noncentrosymmetric Polar Racemate: An Experimental and Theoretical Study. <i>Crystal Growth and Design</i> , 2014, 14, 5822-5833. | 1.4 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8076 | Relating polarizability to volume, ionization energy, electronegativity, hardness, moments of momentum, and other molecular properties. <i>Journal of Chemical Physics</i> , 2014, 141, 074306. | 1.2 | 57 |
| 8077 | Backbiting and \hat{I}^2 -scission reactions in free-radical polymerization of methyl acrylate. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 345-360. | 1.0 | 38 |
| 8078 | A Copper Complex of a Noninnocent Iminophenol- \hat{A} Amidopyridine Hybrid Ligand: Synthesis, Characterization, and Aerobic Alcohol Oxidation. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 6066-6074. | 1.0 | 38 |
| 8079 | The Role of Aryne Distortions, Steric Effects, and Charges in Regioselectivities of Aryne Reactions. <i>Journal of the American Chemical Society</i> , 2014, 136, 15798-15805. | 6.6 | 267 |
| 8080 | Phosphine substitution reactions of (\hat{I} -5-cyclopentadienyl)ruthenium bis(triarylphosphine) chloride, CpRu(PAr ₃) ₂ Cl {PAr ₃ = PPh ₃ , P(p-CH ₃ C ₆ H ₄) ₃ , P(p-FC ₆ H ₄) ₃ , P(p-CH ₃ OC ₆ H ₄) ₃ , and PPh ₂ (p-CH ₃ C ₆ H ₄)}: a tale of two mechanisms. <i>Dalton Transactions</i> , 2014, 43, 15221-15227. | 1.6 | 6 |
| 8081 | The one-electron reduction of dithiolate and diselenolate ligands. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10897. | 1.3 | 11 |
| 8082 | Substrate and product role in the Shvo's catalyzed selective hydrogenation of the platform bio-based chemical 5-hydroxymethylfurfural. <i>Dalton Transactions</i> , 2014, 43, 10224-10234. | 1.6 | 60 |
| 8083 | Kinetics of the NH ₃ and CO ₂ solid-state reaction at low temperature. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 23604-23615. | 1.3 | 27 |
| 8084 | Influence of primary and auxiliary ligand on spectroscopic properties and luminescent efficiency of organoplatinum(\hat{I}) complexes bearing functionalized cyclometalated C ^N C ligands. <i>Dalton Transactions</i> , 2014, 43, 14029. | 1.6 | 10 |
| 8085 | Photoenolization via excited state double proton transfer induces \hat{A} fluorescence in diformyl diaryl dipyrromethane. <i>Chemical Communications</i> , 2014, 50, 8667-8669. | 2.2 | 8 |
| 8086 | Molecular interactions with CO ₂ for controlling the regioselectivity of liquid phase hydrogenation of 2,4-dinitroaniline. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18955-18965. | 1.3 | 2 |
| 8087 | Tuning ligand electronics and peripheral substitution on cobalt salen complexes: structure and polymerisation activity. <i>Dalton Transactions</i> , 2014, 43, 4295-4304. | 1.6 | 66 |
| 8088 | Predicting phosphorescent lifetimes and zero-field splitting of organometallic complexes with time-dependent density functional theory including spin-orbit coupling. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14523-14530. | 1.3 | 155 |
| 8089 | Solvent Effects on Excited-State Structures: A Quantum Monte Carlo and Density Functional Study. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5528-5537. | 2.3 | 12 |
| 8090 | Synergy between experimental and theoretical methods in the exploration of homogeneous transition metal catalysis. <i>Dalton Transactions</i> , 2014, 43, 11093-11105. | 1.6 | 21 |
| 8091 | 1,3,2-Dithiaphospholanes with an annelated 1,2-dicarba-closo-dodecaborane(12) unit: formation and reactivity. <i>Dalton Transactions</i> , 2014, 43, 5021-5043. | 1.6 | 5 |
| 8092 | The reactivity of CO ₂ and H ₂ at trapped electron sites at an oxide surface. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21153-21156. | 1.3 | 8 |
| 8093 | Selective oxidation passing through \hat{I}^3 -ozone intermediates: applications to direct propene epoxidation using molecular oxygen oxidant. <i>RSC Advances</i> , 2014, 4, 27755-27774. | 1.7 | 12 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8094 | Ultrafast photo-induced ligand solvolysis of cis-[Ru(bipyridine) ₂ (nicotinamide) ₂] ²⁺ : experimental and theoretical insight into its photoactivation mechanism. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19141-19155. | 1.3 | 65 |
| 8095 | High nuclearity Ni(ⁱⁱ) cages from hydroxamate ligands. <i>RSC Advances</i> , 2014, 4, 38182-38191. | 1.7 | 15 |
| 8096 | Crystal engineering the clathrate hydrate lattice with NH ₄ F. <i>CrystEngComm</i> , 2014, 16, 7209-7217. | 1.3 | 36 |
| 8097 | A simple BODIPY-aniline-based fluorescent chemosensor as multiple logic operations for the detection of pH and CO ₂ gas. <i>Dalton Transactions</i> , 2014, 43, 8499-8507. | 1.6 | 71 |
| 8098 | A non-Bornian analysis of the Gibbs energy of hydration for organic ions. <i>RSC Advances</i> , 2014, 4, 27634-27641. | 1.7 | 8 |
| 8099 | Modelling excited states of weakly bound complexes with density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14455-14462. | 1.3 | 21 |
| 8100 | Fast and reversible insertion of carbon dioxide into zirconocene-alkoxide bonds. A mechanistic study. <i>Dalton Transactions</i> , 2014, 43, 8894-8898. | 1.6 | 4 |
| 8101 | Effect of metasilicate matrices on boron purification by Amberlite IRA 743 boron specific resin and isotope analysis by MC-ICP-MS. <i>Journal of Analytical Atomic Spectrometry</i> , 2014, 29, 2104-2107. | 1.6 | 7 |
| 8102 | N-Heterocyclic carbene rhodium(ⁱ) complexes containing an axis of chirality: dynamics and catalysis. <i>New Journal of Chemistry</i> , 2014, 38, 1768-1779. | 1.4 | 21 |
| 8103 | Targeting cytotoxicity and tubulin polymerization by metal-carbene complexes on a purine tautomer platform. <i>Dalton Transactions</i> , 2014, 43, 9838-9842. | 1.6 | 15 |
| 8104 | Effect of charge transfer and periodicity on the magnetism of [Cr(Cp*) ₂][ETCE]. <i>RSC Advances</i> , 2014, 4, 14847. | 1.7 | 1 |
| 8105 | All-atom molecular dynamics simulation of HPMA polymers. <i>RSC Advances</i> , 2014, 4, 7003. | 1.7 | 3 |
| 8106 | The reactivity of CO ₂ on the MgO(100) surface. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 184-195. | 1.3 | 36 |
| 8107 | Acidity constants of lumiflavin from first principles molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18993-19000. | 1.3 | 13 |
| 8108 | Through-space charge transfer and emission color tuning of di-o-carborane substituted benzene. <i>Dalton Transactions</i> , 2014, 43, 4978. | 1.6 | 66 |
| 8109 | Formation, structural characterization, and reactions of a unique cyclotrimeric vicinal Lewis pair containing (C ₆ F ₅) ₂ P-Lewis base and (C ₆ F ₅) ₂ BH-Lewis acid components. <i>Dalton Transactions</i> , 2014, 43, 15159-15169. | 1.6 | 15 |
| 8110 | Unusual IR ring mode splittings for pyridinium species in H ₃ PW ₁₂ O ₄₀ heteropolyacid: involvement of the ν_{NH} internal mode. <i>RSC Advances</i> , 2014, 4, 19159-19164. | 1.7 | 2 |
| 8111 | A comparison between QM/MM and QM/QM based fitting of condensed-phase atomic polarizabilities. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17857-17862. | 1.3 | 6 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8112 | One-electron self-interaction and the asymptotics of the Kohn-Sham potential: an impaired relation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14357-14367. | 1.3 | 56 |
| 8113 | Metallo phosphonate catalyzed benzoin couplings: the influence of the counterion. <i>New Journal of Chemistry</i> , 2014, 38, 1040. | 1.4 | 2 |
| 8114 | New supramolecular assemblies in heterobimetallic chemistry: synthesis of a homologous series of unsolvated alkali-metal zincates. <i>Dalton Transactions</i> , 2014, 43, 14229-14238. | 1.6 | 17 |
| 8115 | A new exchange-correlation functional free of delocalization and static correlation errors. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16373-16377. | 1.3 | 3 |
| 8116 | Substrate, Molecular Structure, and Solvent Effects in 2D Self-Assembly via Hydrogen and Halogen Bonding. <i>Journal of Physical Chemistry C</i> , 2014, 118, 25505-25516. | 1.5 | 59 |
| 8117 | Structural, electronic and energetic properties of giant icosahedral fullerenes up to C6000: insights from an ab initio hybrid DFT study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 13390-13401. | 1.3 | 30 |
| 8118 | NO ₂ bond cleavage by MoL ₃ complexes. <i>Dalton Transactions</i> , 2014, 43, 1620-1629. | 1.6 | 3 |
| 8119 | Reaction mechanism and free energy profile for acylation of <i>Candida Antarctica</i> lipase B with methylcaprylate and acetylcholine: Density functional theory calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 54, 131-140. | 1.3 | 10 |
| 8120 | Configurational and energy study of the (100) and (110) surfaces of the MgAl ₂ O ₄ spinel by means of quantum mechanical and empirical techniques. <i>CrystEngComm</i> , 2014, 16, 9224-9235. | 1.3 | 10 |
| 8121 | Syntheses of mono- and diacylated bipyrrroles with rich substitution modes and development of a prodigiosin derivative as a fluorescent Zn(II) probe. <i>RSC Advances</i> , 2014, 4, 6133. | 1.7 | 23 |
| 8122 | Theoretical study of small sodium-potassium alloy clusters through genetic algorithm and quantum chemical calculations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 8895-8904. | 1.3 | 11 |
| 8123 | Solvation chemical shifts of perylenic antenna molecules from molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22309-22320. | 1.3 | 7 |
| 8124 | Conformational, Spectroscopic, and Molecular Dynamics DFT Study of Precursors for New Potential Antibacterial Fluoroquinolone Drugs. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9540-9551. | 1.1 | 26 |
| 8125 | Selective Zn ²⁺ sensing using a modified bipyridine complex. <i>RSC Advances</i> , 2014, 4, 25605. | 1.7 | 24 |
| 8126 | The Redox Chemistry of [Co ₆ C(CO) ₁₅] ²⁺ : A Synthetic Route to New Co-Carbide Carbonyl Clusters. <i>Inorganic Chemistry</i> , 2014, 53, 3818-3831. | 1.9 | 12 |
| 8127 | Diruthenium-Polyyn-diyl Diruthenium Wires: Electronic Coupling in the Long Distance Regime. <i>Journal of the American Chemical Society</i> , 2014, 136, 12174-12183. | 6.6 | 103 |
| 8128 | Do Excited Silicon-Oxygen Double Bonds Emit Light?. <i>Journal of Physical Chemistry C</i> , 2014, 118, 7669-7677. | 1.5 | 26 |
| 8129 | Observation of Water Separated Ion-Pairs between Cations and Phospholipid Headgroups. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4397-4403. | 1.2 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8130 | Ab Initio Study of Charge Transfer between Lithium and Aromatic Hydrocarbons. Can the Results Be Directly Transferred to the Lithium-Graphene Interaction?. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7044-7051. | 1.1 | 5 |
| 8131 | ...Aromaticity and Three-Dimensional Aromaticity: Two sides of the Same Coin?. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 12191-12195. | 7.2 | 242 |
| 8132 | Unraveling the Polymorphism of [(p-cymene)Ru(^η -INA)Cl ₂] through Dispersion-Corrected DFT and NMR GIPAW Calculations. <i>Inorganic Chemistry</i> , 2014, 53, 7926-7935. | 1.9 | 11 |
| 8133 | Introducing a New Azoaromatic Pincer Ligand. Isolation and Characterization of Redox Events in Its Ferrous Complexes. <i>Inorganic Chemistry</i> , 2014, 53, 4678-4686. | 1.9 | 46 |
| 8134 | Reactions of 1,3,2-Diselenaphospholanes with Lewis Acids: Borane and (Pentamethylcyclopentadienyl)rhodium and -iridium Dichloride. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 4865-4876. | 1.0 | 7 |
| 8135 | Ligand Effects on the Regioselectivity of Rhodium-Catalyzed Hydroformylation: Density Functional Calculations Illuminate the Role of Long-Range Noncovalent Interactions. <i>Organometallics</i> , 2014, 33, 4183-4191. | 1.1 | 47 |
| 8136 | DFT Studies on Cu-Catalyzed Cross-Coupling of Diazo Compounds with Trimethylsilylethyne and tert-Butylethyne: Formation of Alkynes for Trimethylsilylethyne while Allenes for tert-Butylethyne. <i>Organometallics</i> , 2014, 33, 3941-3949. | 1.1 | 23 |
| 8137 | Experimental and Computational Studies on the Mechanism of Zwitterionic Ring-Opening Polymerization of γ -Valerolactone with N-Heterocyclic Carbenes. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6553-6560. | 1.2 | 57 |
| 8138 | Heteroleptic Cyclometalated Iridium(III) Complexes Supported by Triarylborylpicolinate Ligand: Ratiometric Turn-On Phosphorescence Response upon Fluoride Binding. <i>Inorganic Chemistry</i> , 2014, 53, 8672-8680. | 1.9 | 43 |
| 8139 | Computational Investigation of Alkynols and Alkyndiols Hydrogenation on a Palladium Cluster. <i>Journal of Physical Chemistry C</i> , 2014, 118, 551-558. | 1.5 | 19 |
| 8140 | Accurate Oxidation Potentials of 40 Benzene and Biphenyl Derivatives with Heteroatom Substituents. <i>Journal of Organic Chemistry</i> , 2014, 79, 9297-9304. | 1.7 | 40 |
| 8141 | Numerical Methods for a Kohn-Sham Density Functional Model Based on Optimal Transport. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4360-4368. | 2.3 | 24 |
| 8142 | Magnetic Anisotropy and Mechanism of Magnetic Relaxation in Er(III) Single-Ion Magnets. <i>Inorganic Chemistry</i> , 2014, 53, 10835-10845. | 1.9 | 86 |
| 8143 | Interactive Chemical Reactivity Exploration. <i>ChemPhysChem</i> , 2014, 15, 3301-3319. | 1.0 | 47 |
| 8144 | Solvatochromic Shift of Brookers' Merocyanine: Hartree-Fock Exchange in Time Dependent Density Functional Calculation and Hydrogen Bonding Effect. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4535-4547. | 2.3 | 24 |
| 8145 | 3,4-Polymerization of Isoprene by Using NSN- and NPN-Ligated Rare Earth Metal Precursors: Switching of Stereo Selectivity and Mechanism. <i>Macromolecules</i> , 2014, 47, 4971-4978. | 2.2 | 70 |
| 8146 | Photoelectron Spectroscopy of Co ₂ H ₂ ⁺ and Density Functional Study of Co _n C ₂ H ₂ (n = 1-3) Anion and Neutral Clusters. <i>Journal of Physical Chemistry A</i> , 2014, 118, 6757-6762. | 1.1 | 7 |
| 8147 | Argentophilicity as Essential Driving Force for a Dynamic Cation-Cation Host-Guest System: [Ag(acetonitrile) ₂] ⁺ ·[Ag ₂ (bis-NHC) ₂] ²⁺ (NHC = N-Heterocyclic Carbene). <i>Inorganic Chemistry</i> , 2014, 53, 10654-10659. | 1.9 | 31 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8148 | Experimental and computational studies of two antibacterial drugs as corrosion inhibitors for mild steel in acid media. <i>Materials and Corrosion - Werkstoffe Und Korrosion</i> , 2014, 65, 935-942. | 0.8 | 57 |
| 8149 | Unexpected DNA Affinity and Sequence Selectivity through Core Rigidity in Guanidinium-Based Minor Groove Binders. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 7663-7672. | 2.9 | 28 |
| 8150 | What Dominates the Error in the CaO Diatomic Bond Energy Predicted by Various Approximate Exchange-Correlation Functionals?. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2291-2305. | 2.3 | 17 |
| 8151 | Conformational Mobility and Pendant Base Effects on Electrochemistry of Synthetic Analogues of the [FeFe]-Hydrogenase Active Site. <i>Organometallics</i> , 2014, 33, 4747-4755. | 1.1 | 47 |
| 8152 | Mechanism of the Decay of Thymine Triplets in DNA Single Strands. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1616-1622. | 2.1 | 38 |
| 8153 | Eleven-Membered Fused Ring Low Band-Gap Polymer with Enhanced Charge Carrier Mobility and Photovoltaic Performance. <i>Advanced Functional Materials</i> , 2014, 24, 3631-3638. | 7.8 | 99 |
| 8154 | Attachment Chemistry of PCBM to a Primary-Amine-Terminated Organic Monolayer on a Si(111) Surface. <i>Langmuir</i> , 2014, 30, 5105-5114. | 1.6 | 11 |
| 8155 | Double Level Selection in a Constitutional Dynamic Library of Coordination Driven Supramolecular Polygons. <i>Inorganic Chemistry</i> , 2014, 53, 7276-7287. | 1.9 | 31 |
| 8156 | DFT study of the single electron transfer mechanisms in Ni-Catalyzed reductive cross-coupling of aryl bromide and alkyl bromide. <i>Journal of Organometallic Chemistry</i> , 2014, 770, 130-135. | 0.8 | 32 |
| 8157 | Proton-Coupled Electron Transfer and Adduct Configuration Are Important for C4a-Hydroperoxyflavin Formation and Stabilization in a Flavoenzyme. <i>Journal of the American Chemical Society</i> , 2014, 136, 241-253. | 6.6 | 65 |
| 8158 | Reliability of Density Functional and Perturbation Theories for Calculating Core-Ionization Spectra of Free Radicals. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2333-2343. | 2.3 | 14 |
| 8159 | Density Functional Theory Study of the Mechanisms of Iron-Catalyzed Aminohydroxylation Reactions. <i>Organometallics</i> , 2014, 33, 1423-1430. | 1.1 | 13 |
| 8160 | Effects of chalcogen substitution on electronic properties and chemical bondings of delafossite CuAlO ₂ . <i>Physica Status Solidi (B): Basic Research</i> , 2014, 251, 1630-1634. | 0.7 | 11 |
| 8161 | Highly Efficient Intrinsic Phosphorescence from a π -Conjugated Poly(silylene) Polymer. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22923-22934. | 1.5 | 6 |
| 8162 | Femtosecond Spectroscopy of Superfluorescent Fluorenyl Benzothiadiazoles with Large Two-Photon and Excited-State Absorption. <i>Journal of Physical Chemistry C</i> , 2014, 118, 13790-13800. | 1.5 | 20 |
| 8163 | Vibrationally Resolved Photoelectron Imaging of Au ₃ H ⁺ . <i>Journal of Physical Chemistry A</i> , 2014, 118, 1031-1037. | 1.1 | 2 |
| 8164 | Photo-stable substituted dihydroindolo[2,3-b]carbazole-based organic dyes: tuning the photovoltaic properties by optimizing the π -structure for panchromatic DSSCs. <i>Tetrahedron</i> , 2014, 70, 8122-8128. | 1.0 | 12 |
| 8165 | Efficient Calculations of Molecular Linear Response Properties for Spectral Regions. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2449-2455. | 2.3 | 51 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8166 | Mechanistic Insight into the Rhodium-Catalyzed O ¹⁶ H Insertion Reaction: A DFT Study. <i>Organometallics</i> , 2014, 33, 2448-2456. | 1.1 | 36 |
| 8167 | Functionalization of aliphatic polyesters by nitroxide radical coupling. <i>Polymer Chemistry</i> , 2014, 5, 5656. | 1.9 | 20 |
| 8168 | Characteristic Spectral Patterns in the Carbon-13 Nuclear Magnetic Resonance Spectra of Hexagonal and Crenellated Graphene Fragments. <i>ChemPhysChem</i> , 2014, 15, 1799-1808. | 1.0 | 11 |
| 8169 | Hypercubane: DFT-based prediction of an O-symmetric double-shell hydrocarbon. <i>Chemical Physics Letters</i> , 2014, 612, 198-202. | 1.2 | 11 |
| 8170 | Effective Ion Mobility Calculations for Macromolecules by Scattering on Electron Clouds. <i>Journal of Physical Chemistry A</i> , 2014, 118, 6763-6772. | 1.1 | 35 |
| 8171 | Theoretical study of 11-thiocyanatoundecanoic acid phenylamide derivatives on corrosion inhibition efficiencies. <i>Canadian Journal of Chemistry</i> , 2014, 92, 876-887. | 0.6 | 5 |
| 8172 | Computational study of singlet and triplet sulfonylnitrenes insertion into the C=C or C-H bonds of ethylene. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 794-802. | 0.9 | 5 |
| 8173 | QTAIM Analysis in the Context of Quasirelativistic Quantum Calculations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4830-4841. | 2.3 | 51 |
| 8174 | Solvation at Surfaces and Interfaces: A Quantum-Mechanical/Continuum Approach Including Nonelectrostatic Contributions. <i>Journal of Physical Chemistry C</i> , 2014, 118, 4715-4725. | 1.5 | 20 |
| 8175 | Polaron Structure and Transport in Fullerene Materials: Insights from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 21785-21797. | 1.5 | 6 |
| 8176 | Approach for Predicting the Standard Free Energy Solvation of H ⁺ and Acidity Constant in Nonaqueous Organic Solvents. <i>Journal of Chemical & Engineering Data</i> , 2014, 59, 3555-3564. | 1.0 | 12 |
| 8177 | SERS as a Probe of Charge-Transfer Pathways in Hybrid Dye/Molecule-Metal Oxide Complexes. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3774-3782. | 1.5 | 25 |
| 8178 | Quantum Chemical Calculations of X-ray Emission Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4557-4564. | 2.3 | 43 |
| 8179 | Molecular Dynamics of Methanol Monocation (CH ₃ OH ⁺) in Strong Laser Fields. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1769-1776. | 1.1 | 11 |
| 8180 | NHC Copper(I) Complexes Bearing Dipyridylamine Ligands: Synthesis, Structural, and Photoluminescent Studies. <i>Inorganic Chemistry</i> , 2014, 53, 9181-9191. | 1.9 | 96 |
| 8181 | Stereoselectivity in Asymmetric Catalysis: The Case of Ruthenium-Catalyzed Ketone Hydrogenation. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2427-2435. | 2.3 | 27 |
| 8182 | A significant role of Arg41 residue in the enzymatic reaction of haloacid dehalogenase I-DEX YL studied by QM/MM method. <i>Journal of Molecular Catalysis B: Enzymatic</i> , 2014, 110, 23-31. | 1.8 | 8 |
| 8183 | Molecular design of new P3HT derivatives: Adjusting electronic energy levels for blends with PCBM. <i>Materials Chemistry and Physics</i> , 2014, 148, 923-932. | 2.0 | 25 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8184 | Explanation of the Source of Very Large Errors in Many Exchangeâ€‘Correlation Functionals for Vanadium Dimer. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2399-2409. | 2.3 | 25 |
| 8185 | Experimental (FT-IR, FT-Raman, UVâ€‘Vis, ¹ H and ¹³ CNMR) and computational (density functional theory) studies on 3-bromophenylboronic acid. <i>Journal of Molecular Structure</i> , 2014, 1076, 358-372. | 1.8 | 21 |
| 8186 | Dinickelametalloenes: Sandwich Compounds of the First-Row Transition Metals (M = Fe, Co, Ni) with Two Pentahapto Planar Nickelacycle Ligands. <i>Organometallics</i> , 2014, 33, 4410-4416. | 1.1 | 11 |
| 8187 | Toward a Robust Quantum-Chemical Description of Organic Mixed-Valence Systems. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3925-3934. | 1.5 | 23 |
| 8188 | Role of Acetate and Water in the Water-Assisted Pd(OAc) ₂ -Catalyzed Cross-Coupling of Alkenes with <i>N</i> -Tosyl Hydrazones: A DFT Study. <i>Organometallics</i> , 2014, 33, 3453-3463. | 1.1 | 22 |
| 8189 | Electronic Circular Dichroism of the Chiral Rigid Tricyclic Dilactam with Nonplanar Tertiary Amide Groups. <i>Journal of Physical Chemistry B</i> , 2014, 118, 11100-11108. | 1.2 | 4 |
| 8190 | Structural and Spectroscopic Characterization of Tinâ€‘Tin Double Bonds in Cyclic Distannenes. <i>Organometallics</i> , 2014, 33, 3904-3918. | 1.1 | 23 |
| 8191 | How Method-Dependent Are Calculated Differences between Vertical, Adiabatic, and Oâ€‘0 Excitation Energies?. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4157-4171. | 1.1 | 74 |
| 8192 | Reaction Dynamics of the 4-Methylphenyl Radical (<i>p</i> -Tolyl) with 1,2-Butadiene (1-Methylallene): Are Methyl Groups Purely Spectators?. <i>Journal of Physical Chemistry A</i> , 2014, 118, 6181-6190. | 1.1 | 7 |
| 8193 | CH ₂ NH ₂ + O ₂ and CH ₃ CHNH ₂ + O ₂ Reaction Kinetics: Photoionization Mass Spectrometry Experiments and Master Equation Calculations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2176-2186. | 1.1 | 52 |
| 8194 | Structures, Vibrational Frequencies, and Stabilities of Halogen Cluster Anions and Cations, X _n ⁺ , <i>n</i> = 3, 4, and 5. <i>Inorganic Chemistry</i> , 2014, 53, 8136-8146. | 1.9 | 13 |
| 8195 | Hydrogen-bonded diketopyrrolopyrrole (DPP) pigments as organic semiconductors. <i>Organic Electronics</i> , 2014, 15, 3521-3528. | 1.4 | 99 |
| 8196 | Simulations of dissociation constants in low pressure supercritical water. <i>Molecular Physics</i> , 2014, 112, 2235-2240. | 0.8 | 4 |
| 8197 | Multilithiation Effect on the First Hyperpolarizability of Carbonâ€‘Boronâ€‘Nitride Heteronanotubes: Activating Segment versus Connecting Pattern. <i>Journal of Physical Chemistry C</i> , 2014, 118, 14185-14191. | 1.5 | 33 |
| 8198 | Charge-constrained auxiliary-density-matrix methods for the Hartreeâ€‘Fock exchange contribution. <i>Journal of Chemical Physics</i> , 2014, 141, 094104. | 1.2 | 21 |
| 8199 | Polarizabilities from Long-Range Corrected DFT Calculations. <i>Journal of Chemical & Engineering Data</i> , 2014, 59, 3160-3166. | 1.0 | 10 |
| 8200 | In Silico Spectroscopy of Tryptophan and Tyrosine Radicals Involved in the Long-Range Electron Transfer of Cytochrome c Peroxidase. <i>Journal of Physical Chemistry B</i> , 2014, 118, 9525-9537. | 1.2 | 12 |
| 8201 | High Chemoselectivity of an Advanced Iron Catalyst for the Hydrogenation of Aldehydes with Isolated Câ€‘C Bond: A Computational Study. <i>Journal of Organic Chemistry</i> , 2014, 79, 9355-9364. | 1.7 | 14 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8202 | Ab Initio Calculations of the Main Crystal Surfaces of Forsterite (Mg ₂ SiO ₄): A Preliminary Study to Understand the Nature of Geochemical Processes at the Olivine Interface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 2498-2506. | 1.5 | 48 |
| 8203 | A Theoretical Study on Hydrogen-Bonded Complex of Proflavine Cation and Water: The Site-Dependent Feature of Hydrogen Bond Strengthening and Weakening. <i>Journal of the Chinese Chemical Society</i> , 2014, 61, 1199-1204. | 0.8 | 17 |
| 8204 | Trinuclear Complexes and Coordination Polymers of Redox-Active Guanidino-Functionalized Aromatic (GFA) Compounds with a Triphenylene Core. <i>Inorganic Chemistry</i> , 2014, 53, 9876-9896. | 1.9 | 23 |
| 8205 | Benchmarking dispersion and geometrical counterpoise corrections for cost-effective large-scale DFT calculations of water adsorption on graphene. <i>Journal of Computational Chemistry</i> , 2014, 35, 1789-1800. | 1.5 | 24 |
| 8206 | Neutral, Cationic, and Anionic Low-Spin Iron(III) Complexes Stabilized by Amidophenolate and Iminobenzosemiquinonate Radical in <i>N</i> , <i>N</i> , <i>O</i> Ligands. <i>Inorganic Chemistry</i> , 2014, 53, 36-48. | 1.9 | 62 |
| 8207 | Using Metallic Noncontact Atomic Force Microscope Tips for Imaging Insulators and Polar Molecules: Tip Characterization and Imaging Mechanisms. <i>ACS Nano</i> , 2014, 8, 5339-5351. | 7.3 | 36 |
| 8208 | Oxygen-Sulfur Exchange and the Gas-Phase Reactivity of Cobalt Sulfide Cluster Anions with Molecular Oxygen. <i>Journal of Physical Chemistry A</i> , 2014, 118, 8163-8169. | 1.1 | 7 |
| 8209 | Theoretical Studies on a New Class of C-C Bond Formation: Palladium-Catalyzed Reactions of \pm -Diazocarbonyl Compounds with Allylic Esters. <i>Organometallics</i> , 2014, 33, 1404-1415. | 1.1 | 25 |
| 8210 | Lifetimes of carbocations encountered along reaction coordinates for terpene formation. <i>Chemical Science</i> , 2014, 5, 3301. | 3.7 | 33 |
| 8211 | Density Differences in Embedding Theory with External Orbital Orthogonality. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9182-9200. | 1.1 | 36 |
| 8212 | Magnetic exchange in {Gd ^{III} -radical} complexes: method assessment, mechanism of coupling and magneto-structural correlations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14568-14577. | 1.3 | 73 |
| 8213 | Resonantly Enhanced Multiphoton Ionization Spectrum of the Neutral Green Fluorescent Protein Chromophore. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3588-3592. | 2.1 | 18 |
| 8214 | Structure-Activity Relationships in Cytotoxic Au ^I /Au ^{III} Complexes Derived from 2-(2-Pyridyl)benzimidazole. <i>Inorganic Chemistry</i> , 2014, 53, 4068-4080. | 1.9 | 21 |
| 8215 | The (100), (111) and (110) surfaces of diamond: an ab initio B3LYP study. <i>Molecular Physics</i> , 2014, 112, 1030-1039. | 0.8 | 55 |
| 8216 | Catalyst activation and the dimerization energy of alkylaluminium compounds. <i>Journal of Organometallic Chemistry</i> , 2014, 772-773, 161-171. | 0.8 | 59 |
| 8217 | A Combined Computational and Spectroelectrochemical Study of Platinum-Bridged Bis-Triarylamine Systems. <i>Inorganic Chemistry</i> , 2014, 53, 1544-1554. | 1.9 | 43 |
| 8218 | Theoretical investigation on the mechanism of FeCl ₃ -catalysed cross-coupling reaction of alcohols with alkenes. <i>Molecular Physics</i> , 2014, 112, 2107-2113. | 0.8 | 1 |
| 8219 | Analytic cubic and quartic force fields using density-functional theory. <i>Journal of Chemical Physics</i> , 2014, 140, 034103. | 1.2 | 38 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8220 | Theoretical study on the mechanism and kinetics of ring-opening polymerization of cyclic esters initiated by tin(II) n-butoxide. Computational and Theoretical Chemistry, 2014, 1044, 29-35. | 1.1 | 30 |
| 8221 | Molecular size from moments of the momentum density. Chemical Physics Letters, 2014, 609, 113-116. | 1.2 | 7 |
| 8222 | Theoretical study on the nickel(0)-mediated coupling of carbon dioxide and benzylidenecyclopropane: Mechanism and selectivity. Computational and Theoretical Chemistry, 2014, 1044, 44-54. | 1.1 | 5 |
| 8223 | Aerobic Carbon-Carbon Bond Cleavage of Alkenes to Aldehydes Catalyzed by First-Row Transition-Metal-Substituted Polyoxometalates in the Presence of Nitrogen Dioxide. Journal of the American Chemical Society, 2014, 136, 10941-10948. | 6.6 | 77 |
| 8224 | Organic Electronic Materials: Recent Advances in the DFT Description of the Ground and Excited States Using Tuned Range-Separated Hybrid Functionals. Accounts of Chemical Research, 2014, 47, 3284-3291. | 7.6 | 324 |
| 8225 | Theoretical unification of hybrid-DFT and $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mtext} \rangle \text{DFT} \langle \text{mml:mtext} \rangle \langle \text{mml:mo} \rangle \hat{\%} \langle \text{mml:mo} \rangle \langle \text{mml:mo} \rangle \# \langle \text{mml:mo} \rangle$ for the treatment of localized orbitals. Physical Review B, 2014, 90, . | | |
| 8226 | Alkenyl-substituted titanocene dichloride complexes: Stability studies, binding and cytotoxicity. Journal of Organometallic Chemistry, 2014, 769, 46-57. | 0.8 | 6 |
| 8227 | The enhanced efficiency to 3.6% based on organic dye as donor and Si/TiO ₂ acceptor bulk hetero-junction solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 292, 1-9. | 2.0 | 18 |
| 8228 | $\langle i \rangle \langle /i \rangle$ -Ylide and $\langle i \rangle \langle /i \rangle$ -Complex Formation in Reactions of a Carbene with Dibenzo and Monobenzo Crown Ethers. Journal of Physical Chemistry A, 2014, 118, 6230-6238. | 1.1 | 4 |
| 8229 | Unifying General and Segmented Contracted Basis Sets. Segmented Polarization Consistent Basis Sets. Journal of Chemical Theory and Computation, 2014, 10, 1074-1085. | 2.3 | 232 |
| 8230 | Parametrization of 2,2,2-Trifluoroethanol Based on the Generalized Amber Force Field Provides Realistic Agreement between Experimental and Calculated Properties of Pure Liquid as Well as Water-Mixed Solutions. Journal of Physical Chemistry B, 2014, 118, 10390-10404. | 1.2 | 22 |
| 8231 | Divergent Pathways and Competitive Mechanisms of Metathesis Reactions between $\langle i \rangle \langle /i \rangle$ Arylprop-2-ynyl Esters and Aldehydes: An Experimental and Theoretical Study. Chemistry - A European Journal, 2014, 20, 10360-10370. | 1.7 | 14 |
| 8232 | Theoretical Study on the Stability and Aromaticity of Metallasilapentalynes. Organometallics, 2014, 33, 1845-1850. | 1.1 | 39 |
| 8233 | Reaction Path Following with Sparse Interpolation. Journal of Chemical Theory and Computation, 2014, 10, 2942-2949. | 2.3 | 12 |
| 8234 | Influence of a Bridging Group and the Substitution Effect of Bis(1,2,4-triazine) N-Donor Extractants on Their Interactions with a $\langle \text{sup} \rangle \text{V} \langle \text{sup} \rangle$ Cation. Inorganic Chemistry, 2014, 53, 7848-7860. | 1.9 | 18 |
| 8235 | $\langle \text{sup} \rangle \hat{\%} \langle \text{sup} \rangle \text{C}^*$ Cyclometalated Platinum(II) NHC Complexes with $\langle i \rangle \langle /i \rangle$ -Ketoimine Ligands. Organometallics, 2014, 33, 898-908. | 1.1 | 36 |
| 8236 | Oxo-Exchange of Gas-Phase Uranyl, Neptunyl, and Plutonyl with Water and Methanol. Inorganic Chemistry, 2014, 53, 2163-2170. | 1.9 | 19 |
| 8237 | High-Accuracy Vibrational Computations for Transition-Metal Complexes Including Anharmonic Corrections: Ferrocene, Ruthenocene, and Osmocene as Test Cases. Journal of Chemical Theory and Computation, 2014, 10, 4565-4573. | 2.3 | 46 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8238 | Reactivity for the Diels-Alder Reaction of Cumulenes: A Distortion-Interaction Analysis along the Reaction Pathway. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2638-2645. | 1.1 | 79 |
| 8239 | Time-Resolved IR Spectroscopy of 1,3-Dicyanophenylcyclopentane-1,3-diyl Diradicals: CN Stretching Wavenumber as a Vibrational Signature of Radical Character. <i>Journal of Physical Chemistry B</i> , 2014, 118, 3991-3997. | 1.2 | 10 |
| 8240 | Spin-State Energetics of Heme-Related Models from DFT and Coupled Cluster Calculations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2306-2321. | 2.3 | 93 |
| 8241 | Gold(III) Corroles for High Performance Organic Solar Cells. <i>Advanced Functional Materials</i> , 2014, 24, 4655-4665. | 7.8 | 48 |
| 8242 | Direct Synthesis of High-Valent Aryl-Cu(II) and Aryl-Cu(III) Compounds: Mechanistic Insight into Arene C-H Bond Metalation. <i>Journal of the American Chemical Society</i> , 2014, 136, 6326-6332. | 6.6 | 117 |
| 8243 | Charge Density Discrepancy Between NBO and QTAIM in Single-wall Armchair Carbon Nanotubes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2014, 22, 575-594. | 1.0 | 8 |
| 8244 | 2-Hydroxyterpenylic Acid: An Oxygenated Marker Compound for \pm -Pinene Secondary Organic Aerosol in Ambient Fine Aerosol. <i>Environmental Science & Technology</i> , 2014, 48, 4901-4908. | 4.6 | 32 |
| 8245 | Pyrroloindolone Synthesis via a Cp*Co ^{III} -Catalyzed Redox-Neutral Directed C-H Alkenylation/Annulation Sequence. <i>Journal of the American Chemical Society</i> , 2014, 136, 5424-5431. | 6.6 | 441 |
| 8246 | Reaction Mechanism of Epoxide Cycloaddition to CO ₂ Catalyzed by Salen-M (M = Co, Al). <i>Tetrahedron Letters</i> , 2014, 55, 1164-1168. | 1.1 | 64 |
| 8247 | Synthesis, spectral analysis, X-ray crystal structures and evaluation of chemical reactivity of five new benzimidazole derivatives through experimental and theoretical studies. <i>Journal of Molecular Structure</i> , 2014, 1076, 272-279. | 1.8 | 12 |
| 8248 | A computational (DFT) study on aza-Claisen rearrangement: Effect of temperature, solvent and substitution on activation barrier. <i>Computational and Theoretical Chemistry</i> , 2014, 1046, 42-48. | 1.1 | 4 |
| 8249 | On the stability of the RuCl ₂ (triphenylphosphine) ₂ (amine) complexes: Ligand substituent effects of cyclic and acyclic amines. <i>Polyhedron</i> , 2014, 81, 661-667. | 1.0 | 7 |
| 8250 | Synthesis, Structure, and Photophysical Properties of Blue-Emitting Zinc(II) Complexes with 3-Aryl-Substituted 1-Pyridylimidazo[1,5-a]pyridine Ligands. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 4310-4319. | 1.0 | 44 |
| 8251 | Investigation of ion cluster formation in a pulsed ion mobility spectrometer operating in the negative mode. <i>Sensors and Actuators B: Chemical</i> , 2014, 204, 467-473. | 4.0 | 4 |
| 8252 | Synthesis and characterization of Cu(II), Zn(II) and Fe(II) complexes supported by pyridylamide ligands. <i>Inorganica Chimica Acta</i> , 2014, 421, 465-472. | 1.2 | 9 |
| 8253 | Methanol as a clean and efficient H-transfer reactant for carbonyl reduction: Scope, limitations, and reaction mechanism. <i>Journal of Catalysis</i> , 2014, 317, 206-219. | 3.1 | 70 |
| 8254 | The stability of B ₁₅ N ₁₅ H _x nano-rings is affected by electron delocalization. <i>Computational and Theoretical Chemistry</i> , 2014, 1046, 1-5. | 1.1 | 4 |
| 8255 | Synthesis and chemiluminescent properties of 6,8-diaryl-2-methylimidazo[1,2-a]pyrazin-3(7H)-ones: Systematic investigation of substituent effect at para-position of phenyl group at 8-position. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2014, 293, 12-25. | 2.0 | 21 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8256 | Nickel-Catalyzed Decarboxylative C–P Cross-Coupling of Alkenyl Acids with P(O)H Compounds. <i>Journal of Organic Chemistry</i> , 2014, 79, 8118-8127. | 1.7 | 84 |
| 8257 | Benchmark Torsional Potentials of Building Blocks for Conjugated Materials: Bifuran, Bithiophene, and Biselenophene. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3647-3655. | 2.3 | 41 |
| 8258 | The Catalytic Mechanism of Carboxylesterases: A Computational Study. <i>Biochemistry</i> , 2014, 53, 5820-5829. | 1.2 | 53 |
| 8259 | Crystal structure of a trinuclear complex of zinc(II) with 2,6-Di-tert-butyl-p-quinone 1- α -phthalazinylhydrazone. <i>Journal of Structural Chemistry</i> , 2014, 55, 475-480. | 0.3 | 1 |
| 8260 | Analytical Harmonic Vibrational Frequencies for the Green Fluorescent Protein Computed with ONIOM: Chromophore Mode Character and Its Response to Environment. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 751-766. | 2.3 | 24 |
| 8261 | Amino-Functionalized Pillar[5]arene. <i>Chemistry - A European Journal</i> , 2014, 20, 10996-11004. | 1.7 | 62 |
| 8262 | Chemical Implications of Incompatible Ligand versus Metal Coordination Geometry Preferences. <i>Inorganic Chemistry</i> , 2014, 53, 3039-3047. | 1.9 | 11 |
| 8263 | Theoretical Approaches to Structure and Spectroscopy of Earth Materials. <i>Reviews in Mineralogy and Geochemistry</i> , 2014, 78, 691-743. | 2.2 | 41 |
| 8264 | Analytic Density Functional Theory Calculations of Pure Vibrational Hyperpolarizabilities: The First Dipole Hyperpolarizability of Retinal and Related Molecules. <i>Journal of Physical Chemistry A</i> , 2014, 118, 748-756. | 1.1 | 6 |
| 8265 | Double-hybrid density functionals. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 576-600. | 6.2 | 292 |
| 8266 | Highly efficient SO ₂ capture by phenyl-containing azole-based ionic liquids through multiple-site interactions. <i>Green Chemistry</i> , 2014, 16, 1211-1216. | 4.6 | 95 |
| 8267 | A New Tool To Guide Halofunctionalization Reactions: The Halonium Affinity (<i>HalA</i>) Scale. <i>Journal of the American Chemical Society</i> , 2014, 136, 13355-13362. | 6.6 | 77 |
| 8268 | Electronic Excited States in Amorphous MEH-PPV Polymers from Large-Scale First Principles Calculations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1272-1282. | 2.3 | 30 |
| 8269 | Performance of Density Functional Theory Procedures for the Calculation of Proton-Exchange Barriers: Unusual Behavior of M06-Type Functionals. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3777-3783. | 2.3 | 44 |
| 8270 | Synthesis of Rhenabenzenes from the Reactions of Rhenacyclobutadienes with Ethoxyethyne. <i>Chemistry - A European Journal</i> , 2014, 20, 14885-14899. | 1.7 | 51 |
| 8271 | Alkenes as Chelating Groups in Diastereoselective Additions of Organometallics to Ketones. <i>Organometallics</i> , 2014, 33, 5371-5377. | 1.1 | 3 |
| 8272 | Hybrid Density Functionals for Clusters of Late Transition Metals: Assessing Energetic and Structural Properties. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4408-4416. | 2.3 | 21 |
| 8273 | Range-Separated meta-GGA Functional Designed for Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4297-4306. | 2.3 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8274 | Optimizing Calculations of Electronic Excitations and Relative Hyperpolarizabilities of Electrooptic Chromophores. <i>Accounts of Chemical Research</i> , 2014, 47, 3258-3265. | 7.6 | 164 |
| 8275 | A Quantum Dynamics Study of the Ultrafast Relaxation in a Prototypical Cu(I)â€“Phenanthroline. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9861-9869. | 1.1 | 74 |
| 8276 | Quantum chemical study of the equatorial/axial exchange of different substituents in nitrogen and phosphorous-containing 6-membered rings: Role of charge transfer interactions. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450047. | 1.8 | 1 |
| 8278 | Bis-glycinato complexes of palladium(II): Synthesis, structural determination, and hydrogen bonding interactions. <i>Inorganica Chimica Acta</i> , 2014, 423, 21-30. | 1.2 | 8 |
| 8279 | All the 2p-block elements in a molecule: experimental and theoretical studies of FBNCO and FBNCO+. <i>Chemical Communications</i> , 2014, 50, 13900-13903. | 2.2 | 4 |
| 8280 | Combined Experimental and Computational Approaches To Elucidate the Structures of Silver Clusters inside the ZSM-5 Cavity. <i>Journal of Physical Chemistry C</i> , 2014, 118, 23874-23887. | 1.5 | 23 |
| 8281 | Faraday Rotation in Graphene Quantum Dots: Interplay of Size, Perimeter Type, and Functionalization. <i>Journal of Physical Chemistry C</i> , 2014, 118, 23996-24005. | 1.5 | 17 |
| 8282 | Synthesis and characterization of MHâ€“HOR dihydrogen bonded ruthenium and osmium complexes (I-5-C5H4CH2OH)MH(PPh3)2 (M = Ru, Os). <i>Science China Chemistry</i> , 2014, 57, 1079-1089. | 4.2 | 5 |
| 8283 | Cob(II)alamin: Relativistic DFT Analysis of the EPR Parameters. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2125-2136. | 2.3 | 12 |
| 8284 | First-Principles Calculation of the Optical Properties of an Amphiphilic Cyanine Dye Aggregate. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1012-1023. | 1.1 | 9 |
| 8285 | Computational Rationalization for the Observed Ground-State Multiplicities of Fluorinated Acylnitrenes. <i>Journal of Organic Chemistry</i> , 2014, 79, 8977-8983. | 1.7 | 23 |
| 8286 | Uptake of One and Two Molecules of 1,3-Butadiene by Platinum Bis(dithiolene): A Theoretical Study. <i>Inorganic Chemistry</i> , 2014, 53, 9692-9702. | 1.9 | 16 |
| 8287 | C^{âˆ“S}-N-Cyclometalated Platinum(II) Complexes with Sterically Demanding 1,2-Diarylimidazole Ligands. <i>Organometallics</i> , 2014, 33, 3464-3473. | 1.1 | 22 |
| 8288 | How Small Amounts of Impurities Are Sufficient to Catalyze the Interconversion of Carbonyl Compounds and Iminium Ions, or Is There a Metathesis through 1,3â€“Oxazetidinium Ions? Experiments, Speculations, and Calculations. <i>Helvetica Chimica Acta</i> , 2014, 97, 1177-1203. | 1.0 | 11 |
| 8289 | Understanding the reaction mechanisms of Pd-catalysed oxidation of alcohols and domino oxidationâ€“arylation reactions using phenyl chloride as an oxidant. <i>Organic Chemistry Frontiers</i> , 2014, 1, 1188-1196. | 2.3 | 17 |
| 8290 | Exploring the Influence of the Protein Environment on Metal-Binding Pharmacophores. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 7126-7135. | 2.9 | 29 |
| 8291 | A novel â€œTurn-Onâ€“fluorescent probe for Fâˆ“ detection in aqueous solution and its application in live-cell imaging. <i>Analytica Chimica Acta</i> , 2014, 849, 36-42. | 2.6 | 39 |
| 8292 | Distinguishing between keto-enol and acid-base forms of firefly oxyluciferin through calculation of excited-state equilibrium constants. <i>Journal of Computational Chemistry</i> , 2014, 35, 2184-2194. | 1.5 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8293 | The origin of exo-stereoselectivity of norbornene in hetero Diels-Alder reactions. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 8079-8086. | 1.5 | 14 |
| 8294 | Thermodynamic Study of Chlorobenzonitrile Isomers: A Survey on the Polymorphism, Pseudosymmetry, and the Chloro- π -Cyano Interaction. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1502-1510. | 1.1 | 12 |
| 8295 | Palladium(0)-Catalyzed Carbon-Hydrogen Bond Functionalization for the Synthesis of Indoloquinazolines. <i>Advanced Synthesis and Catalysis</i> , 2014, 356, 1533-1538. | 2.1 | 15 |
| 8296 | Experimental and Theoretical Studies on the Interaction between Isonicotinic Acid Molecules and Silver Nanoclusters. <i>Spectroscopy Letters</i> , 2014, 47, 754-760. | 0.5 | 5 |
| 8297 | BN-Phenanthryne: Cyclotetramerization of an 1,2-Azaborine Derivative. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 9380-9383. | 7.2 | 81 |
| 8298 | Quantum Yields for Photochemical Production of NO ₂ from Organic Nitrates at Tropospherically Relevant Wavelengths. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2756-2764. | 1.1 | 7 |
| 8299 | Theoretical study of linker-type effect in carbazole-based dyes on performances of dye-sensitized solar cells. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 14 |
| 8300 | Effect of a chiral electrostatic cavity on product selection in a reaction with a bifurcating reaction path. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 9 |
| 8301 | Performance of recent density functionals to discriminate between olefin and nitrogen binding to palladium. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 7 |
| 8302 | Comparative study of Gaussian basis sets for calculation of core electron binding energies in first-row hydrides and glycine. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 12 |
| 8303 | NO adsorption and transformation on the BaO surfaces from density functional theory calculations. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 3 |
| 8304 | Theoretical study on the working mechanism of a reversible light-driven rotary molecular motor. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 3 |
| 8305 | Electronic properties of mixed metal rod-like group 13 nitride oligomers [RMNH] ₁₀ and [R ₃ (RMNH) ₉ H ₃] (M=Al, Ga, In; R=CH ₃). <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 4 |
| 8306 | X-Ray Diffraction and DFT Calculation Elucidation of the Jahn-Teller Effect Observed in Mn(dibenzoylmethanato) ₃ . <i>Journal of Chemical Crystallography</i> , 2014, 44, 352-359. | 0.5 | 10 |
| 8307 | A Cs ₂ CO ₃ -mediated simple and selective method for the alkylation and acylation of 3,4-dihydropyrimidin-2(1H)-thiones. <i>Comptes Rendus Chimie</i> , 2014, 17, 1057-1064. | 0.2 | 6 |
| 8308 | Strong enhancement of parity violation effects in chiral uranium compounds. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17043-17051. | 1.3 | 10 |
| 8309 | Investigation of transannular cycloaddition reactions involving furanoxonium ions using DFT calculations. Implications for the origin of plumarellide and rameswaralide and related polycyclic metabolites isolated from corals. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 7270-7278. | 1.5 | 11 |
| 8310 | Structure and Energetics of Li ⁺ (BF ₄) ⁻ , Li ⁺ (FSI) ⁻ , and Li ⁺ (TFSI) ⁻ : Ab Initio and Polarizable Force Field Approaches. <i>Journal of Physical Chemistry B</i> , 2014, 118, 10785-10794. | 1.2 | 31 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8311 | The Effect of the Sulfur Position on the Melting Points of Lipidic 1-Methyl-3-Thiaalkylimidazolium Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2014, 118, 10232-10239. | 1.2 | 21 |
| 8312 | Optical Spectroscopy of the Bulk and Interfacial Hydrated Electron from Ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7507-7515. | 1.1 | 61 |
| 8313 | Fractional Charge Behavior and Band Gap Predictions with the XYG3 Type of Doubly Hybrid Density Functionals. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9201-9211. | 1.1 | 45 |
| 8314 | Acid-catalyzed hydrolysis of lignin β -O-4 linkages in ionic liquid solvents: a computational mechanistic study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 5423. | 1.3 | 55 |
| 8315 | Mechanism for the decomposition of 5-aza-2'-deoxycytidine: a theoretical study using Monte Carlo simulation plus local microhydration model. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 1 |
| 8316 | Performance of density functionals for computation of core electron binding energies in first-row hydrides and glycine. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 11 |
| 8317 | Loss of a C ₂ H _n fragment from pyrene and circumcoronene. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 4 |
| 8318 | 2-Amino-5-alkylidenethiazol-4-ones as promising lipid peroxidation inhibitors. <i>Monatshefte für Chemie</i> , 2014, 145, 945-952. | 0.9 | 10 |
| 8319 | Theoretical insight on novel donor-acceptor exTTF-based dyes for dye-sensitized solar cells. <i>Journal of Molecular Modeling</i> , 2014, 20, 2188. | 0.8 | 3 |
| 8320 | Empty versus filled polyhedra: 11 vertex bare germanium clusters. <i>Journal of Molecular Modeling</i> , 2014, 20, 2193. | 0.8 | 1 |
| 8321 | Host-guest complexes of calix[4]tubes - prediction of ion selectivity by quantum chemical calculations VI. <i>Journal of Molecular Modeling</i> , 2014, 20, 2200. | 0.8 | 18 |
| 8322 | Theoretical insight into the mechanism for the inhibition of the cysteine protease cathepsin B by 1,2,4-thiadiazole derivatives. <i>Journal of Molecular Modeling</i> , 2014, 20, 2254. | 0.8 | 5 |
| 8323 | Rotational Isomers, Intramolecular Hydrogen Bond, and IR Spectra of o-Vinylphenol. <i>Journal of Applied Spectroscopy</i> , 2014, 81, 15-22. | 0.3 | 2 |
| 8324 | Simultaneous Determination of Structures, Vibrations, and Frontier Orbital Energies from a Self-Consistent Range-Separated Hybrid Functional. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2734-2741. | 2.1 | 49 |
| 8325 | Infrared Multiple Photon Dissociation Spectroscopy of a Gas-Phase Oxo-Molybdenum Complex with 1,2-Dithiolene Ligands. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5407-5418. | 1.1 | 11 |
| 8326 | Cobaloxime-Based Artificial Hydrogenases. <i>Inorganic Chemistry</i> , 2014, 53, 8071-8082. | 1.9 | 78 |
| 8327 | All-Carbon, Neutral Analogue of ExB ₄ : A DFT Study of Polycyclic Aromatic Hydrocarbon Binding. <i>Journal of Physical Chemistry A</i> , 2014, 118, 6104-6111. | 1.1 | 13 |
| 8328 | Redox Reactions of Nickel, Copper, and Cobalt Complexes with π -Noninnocent Dithiolate Ligands: Combined in Situ Spectroelectrochemical and Theoretical Study. <i>Organometallics</i> , 2014, 33, 4846-4859. | 1.1 | 29 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8329 | 17O NMR chemical shifts in oxometalates: from the simplest monometallic species to mixed-metal polyoxometalates. <i>Chemical Science</i> , 2014, 5, 2031. | 3.7 | 44 |
| 8330 | Ferromagnetic Coupling in an Fe[C(SiMe ₃) ₃] ₂ /Ferrihydrite Hetero-Mixture Molecular Magnet. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 3178-3183. | 1.0 | 4 |
| 8331 | Fe ^{III} Bipyrrolidine Phenoxide Complexes and Their Oxidized Analogues. <i>Inorganic Chemistry</i> , 2014, 53, 5810-5819. | 1.9 | 14 |
| 8332 | Catalytic Formation of Ammonia from Molecular Dinitrogen by Use of Dinitrogen-Bridged Dimolybdenum-Dinitrogen Complexes Bearing PNP-Pincer Ligands: Remarkable Effect of Substituent at PNP-Pincer Ligand. <i>Journal of the American Chemical Society</i> , 2014, 136, 9719-9731. | 6.6 | 202 |
| 8333 | 7-Azaindol-1-yl(organo)silanes and Their PdCl ₂ Complexes: Pd-Capped Tetrahedral Silicon Coordination Spheres and Paddlewheels with a Pd-Si Axis. <i>Organometallics</i> , 2014, 33, 2479-2488. | 1.1 | 19 |
| 8334 | Structure and Dynamics of Octamethyl-POSS Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5579-5592. | 1.5 | 27 |
| 8335 | The spectroscopic (FT-IR, FT-Raman), MESP, first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 1,5-dimethyl naphthalene by density functional method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 131, 636-646. | 2.0 | 15 |
| 8336 | Alkaline Hydrolysis of Organophosphorus Pesticides: The Dependence of the Reaction Mechanism on the Incoming Group Conformation. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7277-7289. | 1.2 | 43 |
| 8337 | Infrared Photodissociation Spectroscopy of Oxygen-Rich Fe(O ₂) _n (<i>n</i> = 3-5) Cation Complexes. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4519-4526. | 1.1 | 10 |
| 8338 | Theoretical Investigation of the Controlled Metathesis Reactions of Methylruthenium(II) Complexes with Terminal Acetylenes. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 2502-2511. | 1.0 | 7 |
| 8339 | Electronic structure of positive and negative polarons in functionalized dithienylthiazolo[5,4-d]thiazoles: a combined EPR and DFT study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10032. | 1.3 | 15 |
| 8340 | Lithium ionophore VIII as an extraordinarily effective receptor for the strontium cation: Experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2014, 1061, 110-113. | 1.8 | 2 |
| 8341 | Construction of the B88 Exchange-Energy Functional in Two Dimensions. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1837-1842. | 2.3 | 17 |
| 8342 | New Benchmark Set of Transition-Metal Coordination Reactions for the Assessment of Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3092-3103. | 2.3 | 181 |
| 8343 | Radioiodinated Benzyloxybenzene Derivatives: A Class of Flexible Ligands Target to β -Amyloid Plaques in Alzheimer's Brains. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 6030-6042. | 2.9 | 34 |
| 8344 | Chameleonic Nature of Hydroxyheme in Heme Oxygenase and Its Reactivity: A Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2014, 53, 2766-2775. | 1.9 | 5 |
| 8345 | Mechanism of Cu/Pd-Catalyzed Decarboxylative Cross-Couplings: A DFT Investigation. <i>Journal of the American Chemical Society</i> , 2014, 136, 10007-10023. | 6.6 | 88 |
| 8346 | Origin of the Thermodynamic Stability of the Polymorph IV of Crystalline Barbituric Acid: Evidence from Solid-State NMR and Electron Density Analyses. <i>Crystal Growth and Design</i> , 2014, 14, 2763-2772. | 1.4 | 19 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8347 | Spin-Crossover and Massive Anisotropy Switching of 5d Transition Metal Atoms on Graphene Nanoflakes. <i>Nano Letters</i> , 2014, 14, 3364-3368. | 4.5 | 28 |
| 8348 | Nature of Zr-Monosubstituted Monomeric and Dimeric Polyoxometalates in Water Solution at Different pH Conditions: Static Density Functional Theory Calculations and Dynamic Simulations. <i>Inorganic Chemistry</i> , 2014, 53, 778-786. | 1.9 | 22 |
| 8349 | Time-dependent density functional study of UV-visible absorption spectra of small noble metal clusters (Cu, Ag, Au, n = 2-9, 20). <i>RSC Advances</i> , 2014, 4, 13001. | 1.7 | 43 |
| 8350 | Effect of heteroatoms substitution on electronic, photophysical and charge transfer properties of naphtha [2,1-b:6,5-b'€²] difuran analogues by density functional theory. <i>Computational and Theoretical Chemistry</i> , 2014, 1045, 123-134. | 1.1 | 24 |
| 8351 | Catalytic combustion of dichloromethane over NaFAU and HFAU zeolites: a combined experimental and theoretical study. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2014, 112, 249-265. | 0.8 | 7 |
| 8352 | Thermal racemization of spiropyrans: implication of substituent and solvent effects revealed by computational study. <i>Structural Chemistry</i> , 2014, 25, 667-677. | 1.0 | 10 |
| 8353 | Novel dihydrate formation in p-nitrophenylglyoxal. <i>Structural Chemistry</i> , 2014, 25, 1513-1520. | 1.0 | 2 |
| 8354 | Rearrangements Leading to Fragmentations of Hydrocinnamate and Analogous Nitrogen-Containing Anions Upon Collision-Induced Dissociation. <i>Journal of the American Society for Mass Spectrometry</i> , 2014, 25, 388-397. | 1.2 | 9 |
| 8355 | Mechanistic Study on Electron Capture Dissociation of the Oligosaccharide-Mg ²⁺ Complex. <i>Journal of the American Society for Mass Spectrometry</i> , 2014, 25, 1451-1460. | 1.2 | 26 |
| 8356 | FT-IR, FT-Raman spectra and quantum mechanical study of piperidine-3-carboxylic acid and its tautomers, isomers. <i>Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)</i> , 2014, 116, 906-918. | 0.2 | 1 |
| 8357 | Synthesis, photophysical and electrochemical properties of iridium(III) complexes with 2-aryl-1-phenylbenzimidazoles. <i>Russian Journal of Inorganic Chemistry</i> , 2014, 59, 571-577. | 0.3 | 7 |
| 8358 | Synthesis, physicochemical study, and quantum-chemical simulation of hydrazones based on 2-hydrazinoimidazoline. <i>Russian Journal of General Chemistry</i> , 2014, 84, 676-681. | 0.3 | 1 |
| 8359 | Brightly Luminescent Pt(II) Pincer Complexes with a Sterically Demanding Carboranyl-Phenylpyridine Ligand: A New Material Class for Diverse Optoelectronic Applications. <i>Journal of the American Chemical Society</i> , 2014, 136, 9637-9642. | 6.6 | 165 |
| 8360 | Insight into the Mechanism of Graphene Oxide Degradation via the Photo-Fenton Reaction. <i>Journal of Physical Chemistry C</i> , 2014, 118, 10519-10529. | 1.5 | 101 |
| 8361 | Electrochemical Solvent Reorganization Energies in the Framework of the Polarizable Continuum Model. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2091-2102. | 2.3 | 43 |
| 8362 | Unique behaviour of dinitrogen-bridged dimolybdenum complexes bearing pincer ligand towards catalytic formation of ammonia. <i>Nature Communications</i> , 2014, 5, 3737. | 5.8 | 162 |
| 8363 | Dense and narrowly distributed silica-supported rhodium and iridium nanoparticles: Preparation via surface organometallic chemistry and chemisorption stoichiometry. <i>Journal of Catalysis</i> , 2014, 316, 260-269. | 3.1 | 29 |
| 8364 | Unconventional Facile Way to Metallanaphthalenes from Metal Indenyl Complexes Predicted by DFT Calculations: Origin of Their Different Thermodynamics and Tuning Their Kinetics by Substituents. <i>Organometallics</i> , 2014, 33, 2336-2340. | 1.1 | 32 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8365 | Neutral and Cationic Zinc Complexes with N- and S-Donor-Functionalized Cyclopentadienyl Ligands. <i>Organometallics</i> , 2014, 33, 551-560. | 1.1 | 10 |
| 8366 | Photoemission Spectra and Density Functional Theory Calculations of 3d Transition Metalâ€“Aqua Complexes (Tiâ€“Cu) in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6850-6863. | 1.2 | 28 |
| 8367 | Theoretical and Spectroscopic Analysis of <i>N,N</i> -Diphenylurea and <i>N,N</i> -Dimethyl- <i>N,N</i> -diphenylurea Conformations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5304-5315. | 1.1 | 10 |
| 8368 | A DFT study of isomeric conjugated, cross-conjugated and semi-conjugated six-membered heterocyclic mesomeric betaines. <i>Tetrahedron</i> , 2014, 70, 7158-7165. | 1.0 | 30 |
| 8369 | Molecular and Electronic Structure of Cyclic Trinuclear Gold(I) Carbeniate Complexes: Insights for Structure/Luminescence/Conductivity Relationships. <i>Inorganic Chemistry</i> , 2014, 53, 7485-7499. | 1.9 | 32 |
| 8370 | Mechanistic Insight into the Copper-Catalyzed Phosphorylation of Terminal Alkynes: A Combined Theoretical and Experimental Study. <i>Journal of Organic Chemistry</i> , 2014, 79, 6816-6822. | 1.7 | 66 |
| 8371 | Structure Sensitivity of 2-Methyl-3-butyn-2-ol Hydrogenation on Pd: Computational and Experimental Modeling. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3119-3128. | 1.5 | 30 |
| 8372 | Shape and Morphology Effects on the Electronic Structure of TiO ₂ Nanostructures: From Nanocrystals to Nanorods. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 2471-2478. | 4.0 | 22 |
| 8373 | Magnetostructural characterization of copper(II) hydroxide dimers and coordination polymers coordinated to apical isothiocyanate and cyanide-based counteranions. <i>Canadian Journal of Chemistry</i> , 2014, 92, 1021-1030. | 0.6 | 2 |
| 8374 | Insights into the Stability and Structures of Phosphine-Boranes and Their Î±-Metalated Derivatives. <i>Organometallics</i> , 2014, 33, 5283-5294. | 1.1 | 8 |
| 8375 | Deep Red Phosphorescence of Cyclometalated Iridium Complexes by <i>o</i> -Carborane Substitution. <i>Inorganic Chemistry</i> , 2014, 53, 128-138. | 1.9 | 99 |
| 8376 | Interaction between glyphosate and mitochondrial succinate dehydrogenase. <i>Computational and Theoretical Chemistry</i> , 2014, 1043, 54-63. | 1.1 | 17 |
| 8377 | Synthesis, crystal structure, and electronic structure of a copper(II) chloride complex with 9(E)-phenanthrene-9,10-dione[(1Z)-3,3-dimethyl-3,4-dihydroisoquinolin-1(2H)-ylidene]hydrazone [Cu ₂ (L-H)2Cl ₂]. <i>Russian Journal of Inorganic Chemistry</i> , 2014, 59, 927-934. | 0.3 | 3 |
| 8378 | A uniform approach to the description of multicenter bonding. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20514-20523. | 1.3 | 112 |
| 8379 | Influence of Ligand Flexibility on the Electronic Structure of Oxidized Ni ^{III} -Phenoxide Complexes. <i>Inorganic Chemistry</i> , 2014, 53, 10195-10202. | 1.9 | 33 |
| 8380 | Photophysical Properties of Ruthenium(II) Polypyridyl DNA Intercalators: Effects of the Molecular Surroundings Investigated by Theory. <i>Chemistry - A European Journal</i> , 2014, 20, 12901-12909. | 1.7 | 54 |
| 8381 | Structural and Vibrational Properties of the Ordered Y ₂ CaGe ₄ O ₁₂ Germanate: A Periodic Ab Initio Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 8090-8101. | 1.5 | 18 |
| 8382 | Atomic-Scale Perspective of Ultrafast Charge Transfer at a Dyeâ€“Semiconductor Interface. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2753-2759. | 2.1 | 79 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8383 | Roles of Plasmonic Excitation and Protonation on Photoreactions of <i>p</i> -Aminobenzenethiol on Ag Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2014, 118, 6893-6902. | 1.5 | 33 |
| 8384 | Computational design of <i>in vivo</i> biomarkers. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 143202. | 0.7 | 13 |
| 8385 | A General Quantum Mechanically Derived Force Field (QMDF) for Molecules and Condensed Phase Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4497-4514. | 2.3 | 154 |
| 8386 | The Transmetalation Process in Suzuki–Miyaura Reactions: Calculations Indicate Lower Barrier via Boronate Intermediate. <i>ChemCatChem</i> , 2014, 6, 3132-3138. | 1.8 | 68 |
| 8387 | A computational and experimental study of O-glycosylation. Catalysis by human UDP-GalNAc polypeptide:GalNAc transferase-T2. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 2645-2655. | 1.5 | 39 |
| 8388 | Insights on the Origin of the Unusually Large Specific Rotation of (1 <i>S</i> ,4 <i>S</i>)-Norbornenone. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4863-4871. | 1.1 | 31 |
| 8389 | Ultrafast Excited State Dynamics in 9,9- ² -Bifluorenylidene. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5961-5968. | 1.1 | 15 |
| 8390 | Toward Enabling Large-Scale Open-Shell Equation-of-Motion Coupled Cluster Calculations: Triplet States of ¹² -Carotene. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9087-9093. | 1.1 | 11 |
| 8391 | A new fluorescent probe for Al ³⁺ based on rhodamine 6G and its application to bioimaging. <i>Dalton Transactions</i> , 2014, 43, 12624. | 1.6 | 80 |
| 8392 | Dispersion Interaction Stabilizes Sterically Hindered Double Fullerenes. <i>Chemistry - A European Journal</i> , 2014, 20, 13909-13912. | 1.7 | 21 |
| 8393 | Origins of Diastereoselectivity in Lewis Acid Promoted Ketene–Alkene [2 + 2] Cycloadditions. <i>Organic Letters</i> , 2014, 16, 5168-5171. | 2.4 | 28 |
| 8394 | Impact of d-Orbital Occupation on Metal–Carbon Bond Functionalization. <i>Inorganic Chemistry</i> , 2014, 53, 7789-7798. | 1.9 | 12 |
| 8395 | Mechanism of N–H Bond Cleavage of Aniline by a Dearomatized PNP-Pincer Type Phosphaalkene Complex of Iridium(I). <i>Organometallics</i> , 2014, 33, 715-721. | 1.1 | 26 |
| 8396 | Toward Tunable Immobilized Molecular Catalysts: Functionalizing the Methylene Bridge of Bis(N-heterocyclic carbene) Ligands. <i>ChemPlusChem</i> , 2014, 79, 1294-1303. | 1.3 | 27 |
| 8397 | Reaction pathways and free energy profiles for cholinesterase-catalyzed hydrolysis of 6-monoacetylmorphine. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 2214-2227. | 1.5 | 28 |
| 8398 | Competition between carboxylic and phenolic groups for the preferred sites at the periphery of graphene – A DFT study. <i>Carbon</i> , 2014, 80, 405-418. | 5.4 | 24 |
| 8399 | Linearized self-consistent GW approach satisfying the Ward identity. <i>Physical Review A</i> , 2014, 90, . | 1.0 | 8 |
| 8400 | Role of Isolated Acid Sites and Influence of Pore Diameter in the Low-Temperature Dehydration of Ethanol. <i>ACS Catalysis</i> , 2014, 4, 4161-4169. | 5.5 | 39 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8401 | Solubility, Activity Coefficients, and Protonation Sequence of Risedronic Acid. <i>Journal of Chemical & Engineering Data</i> , 2014, 59, 3728-3740. | 1.0 | 14 |
| 8402 | Cl ⁽⁺⁾ Exchange S _N 2 Reaction inside Carbon Nanotubes: C-H and Cl ⁽⁺⁾ Interactions Govern the Course of the Reaction. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5032-5040. | 1.5 | 29 |
| 8403 | Wave Function and Density Functional Theory Studies of Dihydrogen Complexes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3151-3162. | 2.3 | 23 |
| 8404 | Organic dyes with intense light absorption especially suitable for application in thin-layer dye-sensitized solar cells. <i>Chemical Communications</i> , 2014, 50, 13952-13955. | 2.2 | 64 |
| 8405 | Towards a better understanding of magnetic exchange mediated by hydrogen bonds in Mn(III)/Fe(III) salen-type supramolecular dimers. <i>Dalton Transactions</i> , 2014, 43, 15602-15616. | 1.6 | 39 |
| 8406 | Modeling Spin-Forbidden Monomer Self-Initiation Reactions in Spontaneous Free-Radical Polymerization of Acrylates and Methacrylates. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9310-9318. | 1.1 | 34 |
| 8407 | Constrained Bithiazoles: Small Molecule Correctors of Defective F508 CFTR Protein Trafficking. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 6729-6738. | 2.9 | 20 |
| 8408 | Enlarging the System of Phosphorescent (C*) Cyclometalated Platinum(II) NHC Complexes. <i>Inorganic Chemistry</i> , 2014, 53, 6346-6356. | 1.9 | 78 |
| 8409 | Catalytic Hydrogen Evolution by Fe(II) Carbonyls Featuring a Dithiolate and a Chelating Phosphine. <i>Inorganic Chemistry</i> , 2014, 53, 8919-8929. | 1.9 | 39 |
| 8410 | Vibrational spectroscopic studies on 2,3-didehydro-2,3-dideoxythymidine using density functional theory method. <i>Journal of Molecular Structure</i> , 2014, 1059, 185-192. | 1.8 | 2 |
| 8411 | The structure and bonding of mixed component radical cation clusters. <i>Chemical Physics Letters</i> , 2014, 601, 110-115. | 1.2 | 9 |
| 8412 | 8-Hydroxyquinoline Schiff-base compounds as antioxidants and modulators of copper-mediated A β peptide aggregation. <i>Journal of Inorganic Biochemistry</i> , 2014, 139, 106-116. | 1.5 | 76 |
| 8413 | Reliable evaluation of molecular structure of methyl 3-O-nitro- β -D-glucopyranoside and its intermediates by means of solid-state NMR spectroscopy and DFT optimization in the absence of appropriate crystallographic data. <i>Tetrahedron</i> , 2014, 70, 1910-1917. | 1.0 | 3 |
| 8414 | Hybrid functionals applied to perovskites. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 253202. | 0.7 | 81 |
| 8415 | Synthesis and Characterization of a Uranium(II) Monoarene Complex Supported by π -Backbonding. <i>Angewandte Chemie</i> , 2014, 126, 7286-7290. | 1.6 | 28 |
| 8416 | Spectroscopic trends in a series of Re(I) π -diimine complexes as a function of the antenna/photoisomerizable ligands: a TD-DFT and MS-CASPT2 study. <i>Canadian Journal of Chemistry</i> , 2014, 92, 979-986. | 0.6 | 13 |
| 8417 | Synthesis, mesomorphic, photophysical and computational studies of new achiral four-ring unsymmetrical bent-core mesogens and their Copper(II) complexes. <i>Liquid Crystals</i> , 2014, 41, 1367-1381. | 0.9 | 6 |
| 8418 | Experimental and theoretical study of the interaction of volatile amines with zinc porphyrins. <i>Nanotechnologies in Russia</i> , 2014, 9, 136-144. | 0.7 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8419 | Theoretical Design of n-Type Organic Semiconducting Materials Containing Thiazole and Oxazole Frameworks. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3335-3343. | 1.1 | 32 |
| 8420 | Ligand effects on the redox behavior of bimetallic tungsten(0)/ferrocene(II) complexes. <i>Polyhedron</i> , 2014, 72, 50-55. | 1.0 | 3 |
| 8421 | Do phenolic and carboxylic groups coexist at the tips of oxidized single-wall carbon nanotubes (o-SWNTs)? <i>Carbon</i> , 2014, 73, 194-205. | 5.4 | 10 |
| 8422 | Solvent effect on the photo-induced proton transfer in 2-(N-methyl- β -iminoethyl)-phenol. <i>Chemical Physics Letters</i> , 2014, 591, 52-57. | 1.2 | 4 |
| 8423 | Substituent effects on electronic structure and spectral property of Zn(II) complexes based on the OONX ligands: DFT and TDDFT theoretical studies. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2014, 192, 7-12. | 0.8 | 0 |
| 8424 | Convergence of environment polarization effects in multiscale modeling of excitation energies. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 304-311. | 1.1 | 36 |
| 8425 | Inorganic acid-catalyzed tautomerization of vinyl alcohol to acetaldehyde. <i>Chemical Physics Letters</i> , 2014, 592, 330-333. | 1.2 | 58 |
| 8426 | Pentalene as a ligand in hypoelectronic diruthenaboranes and diosmaboranes with surface metal-metal double bonding. <i>Polyhedron</i> , 2014, 71, 133-141. | 1.0 | 0 |
| 8427 | Experimental and theoretical (FT-IR, FT-Raman, UV-vis, NMR) spectroscopic analysis and first order hyperpolarizability studies of non-linear optical material: (2E)-3-[4-(methylsulfanyl)phenyl]-1-(4-nitrophenyl) prop-2-en-1-one using density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 130, 41-53. | 2.0 | 63 |
| 8428 | DFT study of the electronic and charge transfer properties of perfluoroarene-thiophene oligomers. <i>Journal of Saudi Chemical Society</i> , 2014, 18, 574-580. | 2.4 | 20 |
| 8429 | Direct dynamics investigation of the reaction $S(3P) + CH_4 \rightarrow CH_3 + SH(2\hat{1})$. <i>Chemical Physics Letters</i> , 2014, 591, 103-108. | 1.2 | 8 |
| 8430 | Picture change error in quasirelativistic electron/spin density, Laplacian and bond critical points. <i>Chemical Physics</i> , 2014, 438, 37-47. | 0.9 | 14 |
| 8431 | Thermodynamic properties of 1-phenylnaphthalene and 2-phenylnaphthalene. <i>Journal of Chemical Thermodynamics</i> , 2014, 73, 241-254. | 1.0 | 18 |
| 8432 | Structural and electronic properties of aqueous NaCl solutions from ab initio molecular dynamics simulations with hybrid density functionals. <i>Chemical Physics Letters</i> , 2014, 604, 89-96. | 1.2 | 74 |
| 8433 | Modeling of HXeBr in CO ₂ and Xe environments: Structure, energetics and vibrational spectra. <i>Chemical Physics Letters</i> , 2014, 594, 18-22. | 1.2 | 20 |
| 8434 | Photophysical and biological characterization of new cationic cyclometalated M(III) complexes of rhodium and iridium. <i>Journal of Organometallic Chemistry</i> , 2014, 765, 46-52. | 0.8 | 19 |
| 8435 | Electron-correlation based externally predictive QSARs for mutagenicity of nitrated-PAHs in <i>Salmonella typhimurium</i> TA100. <i>Ecotoxicology and Environmental Safety</i> , 2014, 101, 42-50. | 2.9 | 28 |
| 8436 | Facile dearomatisation of porphyrins using palladium-catalysed hydrazination: the 5,15-diiminoporphodimethenes and their redox products. <i>Tetrahedron</i> , 2014, 70, 517-532. | 1.0 | 9 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8437 | Photo-oxidation by laser pulse induced desorption of phthalocyanines. <i>International Journal of Mass Spectrometry</i> , 2014, 365-366, 89-92. | 0.7 | 0 |
| 8438 | Theoretical investigations of the structures and electronic spectra of Zn(II) and Ni(II) complexes with cyclohexylamine-N-dithiocarbamate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 122, 283-287. | 2.0 | 10 |
| 8439 | Charge transfer optical absorption and fluorescence emission of 4-(9-acridyl)julolidine from long-range-corrected time dependent density functional theory in polarizable continuum approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 370-376. | 2.0 | 14 |
| 8440 | Regioselectivity of the intramolecular nucleophilic attack in [RCH ⁺ NCHC ₆ H ₄ Y]: A mass spectrometric and computational study. <i>Journal of Molecular Structure</i> , 2014, 1063, 8-15. | 1.8 | 0 |
| 8441 | Syngonanthus nitens: Why it looks like spun gold. <i>Industrial Crops and Products</i> , 2014, 52, 597-602. | 2.5 | 4 |
| 8442 | Mechanism of Mo-catalyzed C-S cleavage of thiophene. <i>Journal of Organometallic Chemistry</i> , 2014, 749, 275-286. | 0.8 | 5 |
| 8443 | Synthesis and reaction chemistry of boryliridium hydride complexes formed by oxidative addition of catecholborane to iridium(I): Lessons for metal-catalyzed hydroboration. <i>Journal of Organometallic Chemistry</i> , 2014, 750, 86-97. | 0.8 | 9 |
| 8444 | First-principle study of atomic oxygen and nitrogen adsorption on (111) β -cristobalite as a model of thermal protection coverage. <i>Acta Astronautica</i> , 2014, 100, 40-46. | 1.7 | 13 |
| 8445 | Aggregation behavior of dicephalic di-N-oxide surfactants in aqueous solution: Experimental and computational approaches. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2014, 442, 34-41. | 2.3 | 12 |
| 8446 | Comparative experimental and theoretical studies of N-(4-Methylbenzylidene)-N ⁺ -(2-carboxyphenyl)hydrazine novel Schiff base. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 127, 490-497. | 2.0 | 7 |
| 8447 | Assessment of new DFT methods for predicting vibrational spectra and structure of cisplatin: Which density functional should we choose for studying platinum(II) complexes?. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 125, 431-439. | 2.0 | 38 |
| 8448 | Theoretical and experimental investigation of properties, NLO, NBO and NPA analysis. <i>Journal of Molecular Structure</i> , 2014, 1065-1066, 210-222. | 1.8 | 45 |
| 8449 | A simplified time-dependent density functional theory approach for electronic ultraviolet and circular dichroism spectra of very large molecules. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 45-53. | 1.1 | 211 |
| 8450 | Kinetic and Mechanistic Studies of Carbon-to-Metal Hydrogen Atom Transfer Involving Os-Centered Radicals: Evidence for Tunneling. <i>Journal of the American Chemical Society</i> , 2014, 136, 3572-3578. | 6.6 | 25 |
| 8451 | Nitrogen and Sulfur Compounds in Atmospheric Aerosols: A New Parametrization of Polarized Molecular Orbital Model Chemistry and Its Validation against Converged CCSD(T) Calculations for Large Clusters. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3129-3139. | 2.3 | 9 |
| 8452 | Tribenzotriquinacene Receptors for C ₆₀ ...Fullerene Rotors: Towards Chiral Stators for Unidirectionally Operating Nanoratchets. <i>Chemistry - A European Journal</i> , 2014, 20, 9100-9110. | 1.7 | 30 |
| 8453 | Understanding Lanthanoid(III) Hydration Structure and Kinetics by Insights from Energies and Wave functions. <i>Inorganic Chemistry</i> , 2014, 53, 7700-7708. | 1.9 | 82 |
| 8454 | Drug release by pH-responsive molecular tweezers: Atomistic details from molecular modeling. <i>Journal of Computational Chemistry</i> , 2014, 35, 1545-1551. | 1.5 | 2 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8455 | Hydrolysis of DFP and the Nerve Agent (<i>S</i>)-Sarin by DFPase Proceeds along Two Different Reaction Pathways: Implications for Engineering Bioscavengers. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4479-4489. | 1.2 | 42 |
| 8457 | Effect of Electron (De)localization and Pairing in the Electrochemistry of Polyoxometalates: Study of Wellsâ€“Dawson Molybdotungstophosphate Derivatives. <i>Inorganic Chemistry</i> , 2014, 53, 5941-5949. | 1.9 | 12 |
| 8458 | Quantum Monte Carlo Benchmark of Exchange-Correlation Functionals for Bulk Water. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2355-2362. | 2.3 | 39 |
| 8459 | Which conformations make stable crystal structures? Mapping crystalline molecular geometries to the conformational energy landscape. <i>Chemical Science</i> , 2014, 5, 3173-3182. | 3.7 | 148 |
| 8460 | â€“Unconventionalâ€™ Coordination Chemistry by Metal Chelating Fragments in a Metalloprotein Active Site. <i>Journal of the American Chemical Society</i> , 2014, 136, 5400-5406. | 6.6 | 19 |
| 8461 | Understanding $\hat{1},\hat{2}$ -Unsaturated Imine Formation from Amine Additions to $\hat{1},\hat{2}$ -Unsaturated Aldehydes and Ketones: An Analytical and Theoretical Investigation. <i>Journal of Organic Chemistry</i> , 2014, 79, 5163-5172. | 1.7 | 43 |
| 8462 | Mechanism, Reactivity, and Selectivity in Rh(III)-Catalyzed Phosphoryl-Directed Oxidative C-H Activation/Cyclization: A DFT Study. <i>Journal of Organic Chemistry</i> , 2014, 79, 5074-5081. | 1.7 | 45 |
| 8463 | Neutral Nickel Ethylene Oligo- and Polymerization Catalysts: Towards Computational Catalyst Prediction and Design. <i>Chemistry - A European Journal</i> , 2014, 20, 7962-7978. | 1.7 | 20 |
| 8464 | Boron Carboxylate Catalysis of Homoallylboration. <i>Journal of Organic Chemistry</i> , 2014, 79, 4277-4284. | 1.7 | 8 |
| 8465 | Validating computer simulations of enantioselective catalysis; reproducing the large steric and entropic contributions in <i>Candida Antarctica</i> lipase B. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 1387-1399. | 1.5 | 16 |
| 8466 | Experimental and Computational Studies of the Neutral and Reduced States of Indeno[1,2- <i>b</i>]fluorene. <i>Journal of the American Chemical Society</i> , 2014, 136, 9181-9189. | 6.6 | 41 |
| 8467 | Direct Measurement of Acceptor Group Localization on Donor- Acceptor Polymers Using Resonant Auger Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5570-5578. | 1.5 | 13 |
| 8468 | What Factors Influence the Metal- Proton Spin- Spin Coupling Constants in Mercury- and Cadmium-Substituted Rubredoxin?. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4471-4479. | 1.1 | 10 |
| 8469 | Synthesis, Reactivity, and Electronic Structure of a Bioinspired Heterobimetallic [Ni($\hat{1}/4$ -S ₂)Fe] Complex with Disulfur Monoradical character. <i>Organometallics</i> , 2014, 33, 3154-3162. | 1.1 | 3 |
| 8470 | Computational Study on the Vinyl Azide Decomposition. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5038-5045. | 1.1 | 14 |
| 8471 | Substituent Effects on Rates and Torquoselectivities of Electrocyclic Ring-Openings of <i>N</i> -Substituted 2-Azetines. <i>Journal of Organic Chemistry</i> , 2014, 79, 6189-6195. | 1.7 | 15 |
| 8472 | Branching Out from the Bisabolyl Cation. Unifying Mechanistic Pathways to Barbatene, Bazzanene, Chamigrene, Chamipinene, Cumacrene, Cuprenene, Dunnienne, Isobazzanene, Iso- $\hat{3}$ -bisabolene, Isochamigrene, Laurene, Microbiotene, Sesquithujene, Sesquisabinene, Thujopsene, Trichodiene, and Widdradiene Sesquiterpenes. <i>Journal of the American Chemical Society</i> , 2014, 136, 2450-2463. | 6.6 | 95 |
| 8473 | Nuclear Magnetic Shielding Constants from Quantum Mechanical/Molecular Mechanical Calculations Using Polarizable Embedding: Role of the Embedding Potential. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 981-988. | 2.3 | 37 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8474 | Effect of Extended π -Conjugation of the Donor Structure of Organic Dye on the Photovoltaic Performance of Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2014, 118, 16486-16493. | 1.5 | 63 |
| 8475 | Atmospheric Fate of Nitramines: An Experimental and Theoretical Study of the OH Reactions with CH_3NHNO_2 and $(\text{CH}_3)_2\text{NNO}_2$. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3450-3462. | 1.1 | 15 |
| 8476 | Dearomative Indole (3 + 2) Cycloaddition Reactions. <i>Journal of the American Chemical Society</i> , 2014, 136, 6288-6296. | 6.6 | 141 |
| 8477 | Simulation of the Resonance Raman Spectrum for Uracil. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9228-9238. | 1.1 | 12 |
| 8478 | Long wavelength absorbing carbostyrils as test cases for different TDDFT procedures and solvent models. <i>Journal of Molecular Modeling</i> , 2014, 20, 2217. | 0.8 | 6 |
| 8479 | 2-Diphenylaminothiophene as the donor of porphyrin sensitizers for dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2014, 38, 3227-3235. | 1.4 | 47 |
| 8480 | Penetration Barrier of Water through Graphynes TM Pores: First-Principles Predictions and Force Field Optimization. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 751-755. | 2.1 | 84 |
| 8481 | Modeling the Active Site of [NiFe] Hydrogenases and the [NiFeu] Subsite of the C-Cluster of Carbon Monoxide Dehydrogenases: Low-Spin Iron(II) Versus High-Spin Iron(II). <i>Inorganic Chemistry</i> , 2014, 53, 6329-6337. | 1.9 | 16 |
| 8482 | Heats of formation of the amino acids re-examined by means of W1-F12 and W2-F12 theories. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1. | 0.5 | 74 |
| 8483 | Disklike Hepta- and Tridecanuclear Cobalt Clusters. Synthesis, Structures, Magnetic Properties, and DFT Calculations. <i>Inorganic Chemistry</i> , 2014, 53, 5458-5466. | 1.9 | 43 |
| 8484 | Synthesis and Characterization of Binary-Complex Models of Ureas and 1,3-Dicarbonyl Compounds: Deeper Insights into Reaction Mechanisms Using Snap-Shot Structural Analysis. <i>Journal of Organic Chemistry</i> , 2014, 79, 1805-1817. | 1.7 | 36 |
| 8485 | Experimental and Theoretical Insights into the Mechanisms of Sulfate and Sulfamate Ester Hydrolysis and the End Products of Type I Sulfatase Inactivation by Aryl Sulfamates. <i>Journal of Organic Chemistry</i> , 2014, 79, 1995-2005. | 1.7 | 32 |
| 8486 | Two supramolecular complexes of gallium(III) with different adduct ion pairs containing pyridine-2,6-dicarboxylic acid: Syntheses, characterization, crystal structures and computational study. <i>Journal of Structural Chemistry</i> , 2014, 55, 342-352. | 0.3 | 4 |
| 8487 | Mechanistic Insights on the Stereoselective Nucleophilic 1,2-Addition to Sulfinyl Imines. <i>Journal of Organic Chemistry</i> , 2014, 79, 2514-2521. | 1.7 | 18 |
| 8488 | Computational and DNMR Investigation of the Isomerism and Stereodynamics of the 2,2'-Binaphthalene-1,1'-diol Scaffold. <i>Journal of Organic Chemistry</i> , 2014, 79, 3725-3730. | 1.7 | 11 |
| 8489 | Modulation of the 4-aminophthalimide spectral properties by hydrogen bonds in water. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 131, 214-224. | 2.0 | 5 |
| 8490 | Stepwise and concerted dissociative electron transfer onto a π^* -type orbital in polybrominated aromatics. <i>Electrochemistry Communications</i> , 2014, 43, 117-120. | 2.3 | 14 |
| 8491 | Identification of liquid-phase decomposition species and reactions for guanidinium azotetrazolate. <i>Thermochimica Acta</i> , 2014, 590, 51-65. | 1.2 | 13 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8492 | On the impact of intermolecular interactions between the quaternary ammonium ions on interlayer spacing of quat-intercalated montmorillonite: A molecular mechanics and ab-initio study. <i>Applied Clay Science</i> , 2014, 95, 323-339. | 2.6 | 30 |
| 8493 | Infrared, Raman and NMR spectra, conformational stability and vibrational assignment of 7,8-Dihydroxy-4-Methylcoumarin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 871-878. | 2.0 | 4 |
| 8494 | New cyclic oligothiophenes and their co-oligomers derivatives of molecular engineering interest. <i>Synthetic Metals</i> , 2014, 194, 182-192. | 2.1 | 1 |
| 8495 | Substituent effect on supramolecular motifs in series of succinimide polycyclic keto derivatives – Spectroscopic, theoretical and crystallographic studies. <i>Journal of Molecular Structure</i> , 2014, 1074, 695-702. | 1.8 | 3 |
| 8496 | Configurable photochromism of an unsymmetrical dithienylethene derivative by Cu ²⁺ ions or water. <i>Dyes and Pigments</i> , 2014, 111, 1-7. | 2.0 | 15 |
| 8497 | Absolute configuration of 1,5-diazepin-2-ones: A critical test case for density functional theory. <i>Computational and Theoretical Chemistry</i> , 2014, 1044, 15-23. | 1.1 | 4 |
| 8498 | Density functional theory study of the dipole across the P3HT:PCBM complex: the role of polarization and charge transfer. <i>Journal Physics D: Applied Physics</i> , 2014, 47, 215104. | 1.3 | 29 |
| 8499 | A supramolecular approach towards the construction of molecular salts using phosphonic acid and pyrazole. <i>CrystEngComm</i> , 2014, 16, 7777. | 1.3 | 13 |
| 8500 | Boryl Azides in 1,3-Dipolar Cycloadditions. <i>Journal of Organic Chemistry</i> , 2014, 79, 5478-5483. | 1.7 | 16 |
| 8501 | New Approximation to the Third-Order Density. Application to the Calculation of Correlated Multicenter Indices. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3055-3065. | 2.3 | 31 |
| 8502 | Modulating the Electronic Properties of Multimeric Thiophene Oligomers by Utilizing Carbon Nanotube Confinement. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5510-5522. | 1.5 | 25 |
| 8503 | Tuning the Properties of Pd Nanoclusters by Ligand Coatings: Electronic Structure Computations on Phosphine, Thiol, and Mixed Phosphine-Thiol Ligand Shells. <i>Journal of Physical Chemistry C</i> , 2014, 118, 9790-9800. | 1.5 | 20 |
| 8504 | Dye Aggregation and Complex Formation Effects in 7-(Diethylamino)-coumarin-3-carboxylic Acid. <i>Journal of Physical Chemistry C</i> , 2014, 118, 13042-13051. | 1.5 | 29 |
| 8505 | Orbital gap predictions for rational design of organic photovoltaic materials. <i>Organic Electronics</i> , 2014, 15, 1509-1520. | 1.4 | 110 |
| 8506 | Comparative Study on the Solid Electrolyte Interface Formation by the Reduction of Alkyl Carbonates in Lithium ion Battery. <i>Electrochimica Acta</i> , 2014, 136, 274-285. | 2.6 | 48 |
| 8507 | Free-radical selective functionalization of 1,4-naphthoquinones by perfluorodiacyl peroxides. <i>Tetrahedron</i> , 2014, 70, 5298-5309. | 1.0 | 9 |
| 8508 | Synthesis, characterization and DFT study of nickel(II) complexes of a N ₂ O donor Schiff base with different pseudo-halides: Formation of supra-molecular architectures by C-H...N interactions. <i>Polyhedron</i> , 2014, 78, 94-103. | 1.0 | 21 |
| 8509 | Infrared vibrational and electronic transitions in the dibenzopolyacene family. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 130, 639-652. | 2.0 | 11 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8510 | A comparison of carboxypyridine isomers as sensitizers for dye-sensitized solar cells: assessment of device efficiency and stability. <i>Tetrahedron</i> , 2014, 70, 6285-6295. | 1.0 | 27 |
| 8511 | Sulfur as a heteroatom in metallaborane structures: Cyclopentadienylcobalt thiaboranes. <i>Polyhedron</i> , 2014, 78, 130-134. | 1.0 | 3 |
| 8512 | TABS: A database of molecular structures. <i>Computational and Theoretical Chemistry</i> , 2014, 1043, 13-16. | 1.1 | 21 |
| 8513 | First hyperpolarizability orientation in [70]PCBM isomers: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2014, 1038, 1-5. | 1.1 | 30 |
| 8514 | Geometric and electronic structures of B12C6N6 fullerene. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2014, 56, 216-221. | 1.3 | 15 |
| 8515 | Enthalpies of formation of dihydroxybenzenes revisited: Combining experimental and high-level ab initio data. <i>Journal of Chemical Thermodynamics</i> , 2014, 73, 90-96. | 1.0 | 24 |
| 8516 | Theoretical studies on the electronic structures and photoelectron spectra of tri-rhenium oxide clusters: Re_3O and Re_3O ($n = 1\text{--}6$). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 117, 651-657. | 1.1 | 31 |
| 8517 | Structural and spectroscopic properties of Ir(III) complexes with phenylpyridine ligands: Absorption spectra without and with spin-orbit-coupling. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 219-229. | 1.1 | 31 |
| 8518 | Ferrocene-based sulfonyl dihydropyrazole derivatives: Synthesis, structure, electrochemistry and effect on thermal decomposition of NH_4ClO_4 . <i>Journal of Molecular Structure</i> , 2014, 1067, 112-119. | 1.8 | 38 |
| 8519 | X-ray Sources and Detectors. , 2014, , 14-39. | | 0 |
| 8520 | Neutral and charged boron-doped fullerenes for CO_2 adsorption. <i>Beilstein Journal of Nanotechnology</i> , 2014, 5, 413-418. | 1.5 | 29 |
| 8521 | Stereochemistry of Complex Marine Natural Products by Quantum Mechanical Calculations of NMR Chemical Shifts: Solvent and Conformational Effects on Okadaic Acid. <i>Marine Drugs</i> , 2014, 12, 176-192. | 2.2 | 20 |
| 8522 | Towards improved local hybrid functionals by calibration of exchange-energy densities. <i>Journal of Chemical Physics</i> , 2014, 141, 204101. | 1.2 | 68 |
| 8523 | Two-dimensional x-ray correlation spectroscopy of remote core states. <i>Structural Dynamics</i> , 2014, 1, 014101. | 0.9 | 7 |
| 8524 | Design of Fullerene-Free Electron-Acceptor Materials Containing Perylene-dimide Units for Solution-Processed Organic Electronic Devices. <i>Bulletin of the Chemical Society of Japan</i> , 2014, 87, 1083-1093. | 2.0 | 3 |
| 8525 | Kinetics of Hydrogen Abstraction Reactions from Fluoromethanes and Fluoroethanes. <i>Bulletin of the Chemical Society of Japan</i> , 2014, 87, 890-901. | 2.0 | 30 |
| 8526 | Radical Cyclization and 1,5-Hydrogen Transfer in Selected Aromatic Diazonium Salts. <i>Heterocycles</i> , 2014, 89, 83. | 0.4 | 3 |
| 8527 | Modeling OPV Performance—Morphology, Transport and Recombination. , 2014, , 515-554. | | 0 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8528 | Role of the Isolable Hydride Intermediate in the Hydrosilylation of Carbonyl Compounds Catalyzed by the High-Valent Mono-Oxo-Rhenium(V) Complex. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 5714-5723. | 1.0 | 9 |
| 8529 | Designing Molecular Flip-Flops – DFT Investigations on the Enantiomerization of Hetero Helicenes. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2014, 640, 986-993. | 0.6 | 0 |
| 8530 | <i>Diels-Alder</i> Cyclization of a Dihydropyridine: NMR Spectroscopy, X-Ray Crystallography, and DFT Computations. Bent Aromatic Dimeric Clusters in the Solid Phase. <i>Helvetica Chimica Acta</i> , 2014, 97, 1365-1382. | 1.0 | 0 |
| 8531 | Catalytic Effect of Cesium Cation Adduct Formation on the Decarboxylation of Carboxylate Ions in the Gas Phase. <i>Chemistry - A European Journal</i> , 2014, 20, 815-823. | 1.7 | 5 |
| 8532 | Hydrosilylation Induced by Na ⁺ /Si Intramolecular Coordination: Spontaneous Transformation of Organosilanes into 1-Aza-6-Silole-Type Molecules in the Absence of a Catalyst. <i>Chemistry - A European Journal</i> , 2014, 20, 2542-2550. | 1.7 | 23 |
| 8533 | Investigations on the Enantiomerization Mechanism of an Organophosphorus Cages – DFT Study. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2014, 640, 412-416. | 0.6 | 1 |
| 8534 | Theoretical description for the Rh(I)-catalyzed borylation mechanism of a typical aryl cyanide. <i>Journal of Organometallic Chemistry</i> , 2015, 791, 198-203. | 0.8 | 2 |
| 8535 | Kinetics and Mechanism of the Oxidation of Cyclic Methylsiloxanes by Hydroxyl Radical in the Gas Phase: An Experimental and Theoretical Study. <i>Environmental Science & Technology</i> , 2015, 49, 13322-13330. | 4.6 | 84 |
| 8536 | Influence of the number of anchor groups on the photophysical properties of coordination compounds as components of dye-sensitized solar cells. <i>Russian Chemical Bulletin</i> , 2015, 64, 1801-1807. | 0.4 | 3 |
| 8537 | The X1 family of methods that combines B3LYP with neural network corrections for an accurate yet efficient prediction of thermochemistry. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1021-1031. | 1.0 | 18 |
| 8538 | A Combined IM-MS/DFT Study on [Pd(MPAA)]-Catalyzed Enantioselective C-H Activation: Relay of Chirality through a Rigid Framework. <i>Chemistry - A European Journal</i> , 2015, 21, 11180-11188. | 1.7 | 94 |
| 8539 | Preliminary Characterization and In Vivo Studies of Structurally Identical 18F- and 125I-Labeled Benzyloxybenzenes for PET/SPECT Imaging of β -Amyloid Plaques. <i>Scientific Reports</i> , 2015, 5, 12084. | 1.6 | 14 |
| 8540 | Pair Densities in Density Functional Theory. <i>Multiscale Modeling and Simulation</i> , 2015, 13, 1259-1289. | 0.6 | 12 |
| 8542 | Simple screened exact-exchange approach for excitonic properties in solids. <i>Physical Review B</i> , 2015, 92, . | 1.1 | 55 |
| 8543 | Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory. <i>Physical Review B</i> , 2015, 92, . | 1.1 | 210 |
| 8544 | Calibrating transition-metal energy levels and oxygen bands in first-principles calculations: Accurate prediction of redox potentials and charge transfer in lithium transition-metal oxides. <i>Physical Review B</i> , 2015, 92, . | 1.1 | 126 |
| 8545 | Ether Cleavage Reinvestigated: Elucidating the Mechanism of BBr_3 -Facilitated Demethylation of Aryl Methyl Ethers. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 7460-7467. | 1.2 | 40 |
| 8546 | Reproducing kernel potential energy surfaces in biomolecular simulations: Nitric oxide binding to myoglobin. <i>Journal of Chemical Physics</i> , 2015, 143, 105103. | 1.2 | 16 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8547 | Visual Identification of Light-Driven Breakage of the Silver-Dithiocarbamate Bond by Single Plasmonic Nanoprobes. <i>Scientific Reports</i> , 2015, 5, 15427. | 1.6 | 14 |
| 8548 | Long-range correction for tight-binding TD-DFT. <i>Journal of Chemical Physics</i> , 2015, 143, 134120. | 1.2 | 51 |
| 8549 | Electrostatic point charge fitting as an inverse problem: Revealing the underlying ill-conditioning. <i>Journal of Chemical Physics</i> , 2015, 143, 134102. | 1.2 | 5 |
| 8550 | Fast, accurate evaluation of exact exchange: The occ-RI-K algorithm. <i>Journal of Chemical Physics</i> , 2015, 143, 024113. | 1.2 | 44 |
| 8551 | Nuclear velocity perturbation theory for vibrational circular dichroism: An approach based on the exact factorization of the electron-nuclear wave function. <i>Journal of Chemical Physics</i> , 2015, 143, 074106. | 1.2 | 67 |
| 8552 | Study of lattice vibration and thermal conductivity of BiCuSeO from first-principles calculations. <i>Materials Research Society Symposia Proceedings</i> , 2015, 1735, 110. | 0.1 | 0 |
| 8553 | Absolute NMR shielding scales and nuclear spin-rotation constants in ^{175}LuX and ^{197}AuX ($X = \text{19F, Tj ETQq0 0 0 rgBT / Overlock 10}$) | 1.2 | 18 |
| 8554 | The ground-state potential energy curve of the radium dimer from relativistic coupled cluster calculations. <i>Journal of Chemical Physics</i> , 2015, 143, 084307. | 1.2 | 3 |
| 8555 | Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. <i>Journal of Chemical Physics</i> , 2015, 143, 134702. | 1.2 | 84 |
| 8556 | Implementation and benchmark of a long-range corrected functional in the density functional based tight-binding method. <i>Journal of Chemical Physics</i> , 2015, 143, 184107. | 1.2 | 64 |
| 8557 | Assessment of TD-DFT and LF-DFT for study of $\langle i \rangle d \langle i \rangle \hat{a}'' \langle i \rangle d \langle i \rangle$ transitions in first row transition metal hexaaqua complexes. <i>Journal of Chemical Physics</i> , 2015, 142, 214111. | 1.2 | 32 |
| 8558 | Development of bright fluorescent quadracyclic adenine analogues: TDDFT-calculation supported rational design. <i>Scientific Reports</i> , 2015, 5, 12653. | 1.6 | 17 |
| 8559 | The role of cytosine methylation on charge transport through a DNA strand. <i>Journal of Chemical Physics</i> , 2015, 143, 094306. | 1.2 | 9 |
| 8560 | Perspective: Treating electron over-delocalization with the DFT+U method. <i>Journal of Chemical Physics</i> , 2015, 142, 240901. | 1.2 | 154 |
| 8561 | Beyond the electric-dipole approximation: A formulation and implementation of molecular response theory for the description of absorption of electromagnetic field radiation. <i>Journal of Chemical Physics</i> , 2015, 142, 244111. | 1.2 | 48 |
| 8562 | Chemically Robust Phthalocyanines: Photosensitizer and Electron Shuttle in Solid State Dye Sensitized Solar Cells. <i>Materials Research Society Symposia Proceedings</i> , 2015, 1784, 1. | 0.1 | 0 |
| 8563 | Density function theory study on structures and electronic properties of 2Meq2AlOPh and its derivatives. <i>IOP Conference Series: Materials Science and Engineering</i> , 2015, 87, 012104. | 0.3 | 1 |
| 8564 | Fragment-based ^{13}C nuclear magnetic resonance chemical shift predictions in molecular crystals: An alternative to planewave methods. <i>Journal of Chemical Physics</i> , 2015, 143, 102809. | 1.2 | 65 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8565 | Effect of ensemble generalization on the highest-occupied Kohn-Sham eigenvalue. <i>Journal of Chemical Physics</i> , 2015, 143, 104105. | 1.2 | 16 |
| 8566 | Communication: Hole localization in Al-doped quartz SiO ₂ within <i>ab initio</i> hybrid-functional DFT. <i>Journal of Chemical Physics</i> , 2015, 143, 111103. | 1.2 | 32 |
| 8567 | Fragmentation of mercury compounds under ultraviolet light irradiation. <i>Journal of Chemical Physics</i> , 2015, 143, 074307. | 1.2 | 3 |
| 8568 | Reductive functionalization of 3d metal-methyl complexes: The greater importance of ligand than metal. <i>Computational and Theoretical Chemistry</i> , 2015, 1069, 86-95. | 1.1 | 8 |
| 8569 | Evaluation of Hybrid Theoretical Approaches for Structural Determination of a Glycine-Linked Cisplatin Derivative via Infrared Multiple Photon Dissociation (IRMPD) Action Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10980-10987. | 1.1 | 35 |
| 8570 | Photoinduced Br Desorption from CsBr Thin Films Grown on Cu(100). <i>Journal of Physical Chemistry C</i> , 2015, 119, 24036-24045. | 1.5 | 4 |
| 8571 | NO binding kinetics in myoglobin investigated by picosecond Fe K-edge absorption spectroscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 12922-12927. | 3.3 | 30 |
| 8572 | Excited-State Proton Transfer Can Tune the Color of Protein Fluorescent Markers. <i>ChemPhysChem</i> , 2015, 16, 3444-3449. | 1.0 | 18 |
| 8573 | Nickel-Containing Keggin-Type Polyoxometalates as Hydrogen Evolution Catalysts: Photochemical Structure-Activity Relationships. <i>ChemPlusChem</i> , 2015, 80, 1389-1398. | 1.3 | 45 |
| 8574 | Hexaethyl-2,3,5-tricarba-nido-hexaborane(7), Its Monoanion and the (Triphenylphosphane)gold and Dicarbonylrhodium Complexes. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 4101-4107. | 1.0 | 3 |
| 8575 | Diboranyl Phosphonium Cations: Synthesis and Chemical Properties. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 5188-5195. | 1.0 | 15 |
| 8576 | Circular Dichroism and TDDFT Investigation of Chiral Fluorinated Aryl Benzyl Sulfoxides. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 5554-5562. | 1.2 | 14 |
| 8577 | Application of a BOSS-Gaussian interface for QM/MM simulations of H-ery and methyl transfer reactions. <i>Journal of Computational Chemistry</i> , 2015, 36, 2064-2074. | 1.5 | 12 |
| 8578 | Can 2-acylpyrroles form an intramolecular hydrogen bond?. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 652-662. | 0.9 | 3 |
| 8579 | Hydroxylamine synthesis by oxygen insertion into Re ξ ;NH ₂ bond via Baeyer-Villiger oxidation: a Theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 690-694. | 0.9 | 0 |
| 8580 | Origins of regioselectivity in radical arylation of aniline: A computational study. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1658-1667. | 1.0 | 8 |
| 8581 | Cyclometalated Iridium(III) Complexes Containing Semicarbazone Ligands: Synthesis, Characterization, Photophysical and Biological Studies. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2015, 641, 1798-1802. | 0.6 | 6 |
| 8582 | Experimentelle und theoretische Untersuchungen zur katalytischen asymmetrischen 4-Elektrocyclisierung von N-Heterocyclen. <i>Angewandte Chemie</i> , 2015, 127, 2801-2804. | 1.6 | 15 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8583 | Synthesis and EPR/UV/Vis-NIR Spectroelectrochemical Investigation of a Persistent Phosphanyl Radical Dication. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 11054-11058. | 7.2 | 33 |
| 8584 | N-Doped Carbon Networks: Alternative Materials Tracing New Routes for Activating Molecular Hydrogen. <i>Chemistry - A European Journal</i> , 2015, 21, 3806-3814. | 1.7 | 11 |
| 8585 | How a Redox-Innocent Metal Promotes the Formal Reductive Elimination of Biphenyl Using Redox-Active Ligands. <i>Chemistry - A European Journal</i> , 2015, 21, 4308-4314. | 1.7 | 12 |
| 8586 | Iridicyclic-Catalysed Imine Reduction: An Experimental and Computational Study of the Mechanism. <i>Chemistry - A European Journal</i> , 2015, 21, 16564-16577. | 1.7 | 46 |
| 8587 | Reversal Circularly Polarized Luminescence of Al-Active Chiral Binaphthyl Molecules from Solution to Aggregation. <i>Chemistry - A European Journal</i> , 2015, 21, 13196-13200. | 1.7 | 78 |
| 8588 | From Saturated BN Compounds to Isoelectronic BN/CC Counterparts: An Insight from Computational Perspective. <i>Chemistry - A European Journal</i> , 2015, 21, 15299-15307. | 1.7 | 14 |
| 8589 | Synthesis and Electronic Structure of Ru ₂ (X ₄) ₄ (Y _{gem} -DEE) Type Compounds: Effect of Cross-Conjugation. <i>Inorganic Chemistry</i> , 2015, 54, 7645-7652. | 1.9 | 25 |
| 8590 | Nonspherical Deltahedra in Low-Energy Dicarbalane Structures Testing the Wade-Mingos Rules: The Regular Icosahedron Is Not Favored for the 12-Vertex Dicarbalane. <i>Inorganic Chemistry</i> , 2015, 54, 11377-11384. | 1.9 | 10 |
| 8591 | Synthesis of 4-silaspiro[3.4]octa-1,5-diene derivatives: hybrid spiro compounds. <i>Applied Organometallic Chemistry</i> , 2015, 29, 384-391. | 1.7 | 8 |
| 8592 | Binding of Reactive Oxygen Species at Fe ₄ S Cubane Clusters. <i>Chemistry - A European Journal</i> , 2015, 21, 19081-19089. | 1.7 | 7 |
| 8593 | Estimation of Lattice Enthalpies of Ionic Liquids Supported by Hirshfeld Analysis. <i>ChemPhysChem</i> , 2015, 16, 2890-2898. | 1.0 | 9 |
| 8594 | Azadipyromethene-Based Near-Infrared Dyes: Effect of Thienylethynyl Substitution at the Distal and Proximal Phenyl Groups. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 3649-3657. | 1.0 | 8 |
| 8595 | Simulation of SERS by a DFT study: a comparison of static and near-resonance Raman for 4-mercaptopyridine on small Ag clusters. <i>Journal of Optics (United Kingdom)</i> , 2015, 17, 114004. | 1.0 | 21 |
| 8596 | Controllable Perovskite Crystallization by Water Additive for High-Performance Solar Cells. <i>Advanced Functional Materials</i> , 2015, 25, 6671-6678. | 7.8 | 321 |
| 8597 | The Influence of the Amide Linkage in the Fe ^{III} -Binding Properties of Catechol-Modified Rosamine Derivatives. <i>Chemistry - A European Journal</i> , 2015, 21, 15692-15704. | 1.7 | 8 |
| 8598 | Thermochromism of Cu ^I Tetrakisguanidine Complexes: Reversible Activation of Metal-Ligand Charge-Transfer Bands. <i>Chemistry - A European Journal</i> , 2015, 21, 16494-16503. | 1.7 | 22 |
| 8599 | The Clar Structure in Inorganic BN Analogues of Polybenzenoid Hydrocarbons: Does it Exist or Not?. <i>ChemPhysChem</i> , 2015, 16, 3806-3813. | 1.0 | 16 |
| 8600 | Controlling the Microstructure of Isotactic Polypropene by C ₂ -Symmetric Zirconocene Polymerization Catalysts: Influence of Alkyl Substituents on Regio- and Stereocontrol. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 4420-4428. | 1.0 | 16 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8601 | Structure and stability of supramolecular crown ether complexes. <i>Journal of Computational Chemistry</i> , 2015, 36, 1467-1472. | 1.5 | 7 |
| 8602 | An ab initio Based Structure Property Relationship for Prediction of Ignition Delay of Hypergolic Ionic Liquids. <i>Propellants, Explosives, Pyrotechnics</i> , 2015, 40, 759-764. | 1.0 | 14 |
| 8603 | Electronic structure of a hydrogenated gallium nitride nanoparticle. <i>Physica Status Solidi (B): Basic Research</i> , 2015, 252, 2317-2322. | 0.7 | 1 |
| 8604 | Mechanism of proteolysis in matrix metalloproteinase-2 revealed by QM/MM modeling. <i>Journal of Computational Chemistry</i> , 2015, 36, 1621-1630. | 1.5 | 36 |
| 8605 | Experimental and four-component relativistic DFT studies of tungsten carbonyl complexes. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 723-731. | 0.9 | 17 |
| 8606 | Mechanistic Investigations of the Stereoselective Rare Earth Metal-Mediated Ring-Opening Polymerization of γ -Butyrolactone. <i>Chemistry - A European Journal</i> , 2015, 21, 13609-13617. | 1.7 | 33 |
| 8607 | Intramolecular enantiomerism as revealed from Raman optical activity spectrum. <i>Journal of Raman Spectroscopy</i> , 2015, 46, 1303-1309. | 1.2 | 2 |
| 8608 | First-principle modelling of forsterite surface properties: Accuracy of methods and basis sets. <i>Journal of Computational Chemistry</i> , 2015, 36, 1439-1445. | 1.5 | 14 |
| 8609 | Assessment and acceleration of binding energy calculations for protein-ligand complexes by the fragment molecular orbital method. <i>Journal of Computational Chemistry</i> , 2015, 36, 2209-2218. | 1.5 | 27 |
| 8610 | Conformational analysis of an acyclic tetrapeptide: <i>ab-initio</i> structure determination from X-ray powder diffraction, Hirshfeld surface analysis and electronic structure. <i>Journal of Peptide Science</i> , 2015, 21, 845-852. | 0.8 | 10 |
| 8611 | Coordination of Nickel(II) by 3-(2-(Diphenylphosphanyl)phenyl)acetylpyrazole. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2015, 641, 2093-2101. | 0.6 | 1 |
| 8612 | The B-N Bond in Some Aminoboranes and an Iminoborane, Studied by ^{11}B and ^{15}N NMR Spectroscopy and DFT Methods. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2015, 641, 2525-2529. | 0.6 | 7 |
| 8613 | Germacyclobutenes: Generation by 1,1-Carbalumination or 1,1-Carbagallation and Their Photophysical Properties. <i>Chemistry - A European Journal</i> , 2015, 21, 2629-2637. | 1.7 | 11 |
| 8614 | Intramolecular Communication in Anionic Oxidized Phosphanes through a Chelated Proton. <i>Chemistry - A European Journal</i> , 2015, 21, 8613-8625. | 1.7 | 7 |
| 8615 | Theoretical Characterisation of Phosphinyl Radicals and Their Magnetic Properties: <i>g</i> Matrix. <i>ChemPhysChem</i> , 2015, 16, 1912-1925. | 1.0 | 18 |
| 8616 | Molecular Simulations of Fatty Acid Methyl Esters and Representative Biodiesel Mixtures. <i>ChemPhysChem</i> , 2015, 16, 2810-2817. | 1.0 | 14 |
| 8617 | Extremely Facile Transformations of Tris(3,5-dimethylpyrazolyl)borate: a Bidentate Nitrogen Ligand and a C ₂ -Chiral Cation. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 3232-3235. | 1.0 | 2 |
| 8618 | Dioxygen Activation by an in situ Reduced Cu ^{II} Hydrazone Complex. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 4006-4012. | 1.0 | 6 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8619 | Mechanistic Aspects of a Highly Active Dinuclear Zinc Catalyst for the Co ^{II} -catalyzed Polymerization of Epoxides and CO ₂ . <i>Chemistry - A European Journal</i> , 2015, 21, 8148-8157. | 1.7 | 58 |
| 8620 | Mechanism of Thioether Oxidation over Di ^μ - and Tetrameric Ti Centres: Kinetic and DFT Studies Based on Model Ti-Containing Polyoxometalates. <i>Chemistry - A European Journal</i> , 2015, 21, 14496-14506. | 1.7 | 27 |
| 8621 | New density functional parameterizations to accurate calculations of electric field gradient variations among compounds. <i>Journal of Computational Chemistry</i> , 2015, 36, 2125-2130. | 1.5 | 2 |
| 8622 | Formation of charge-transfer complexes significantly improves the performance of polymer solar cells based on PBDTTT-C-T: PC71 BM. <i>Progress in Photovoltaics: Research and Applications</i> , 2015, 23, 783-792. | 4.4 | 6 |
| 8623 | Iridium-Catalyzed [2+2+2] Cycloaddition of $\text{I}^{\pm}\text{I}^{\pm}$ -Diyne with Cyanamides. <i>Advanced Synthesis and Catalysis</i> , 2015, 357, 3901-3916. | 2.1 | 35 |
| 8625 | Chemical Bonding and Electronic Localization in a Ga ^I Amide. <i>Chemistry - A European Journal</i> , 2015, 21, 14460-14470. | 1.7 | 5 |
| 8626 | Ruthenium-Grafted Vinylhelicenes: Chiroptical Properties and Redox Switching. <i>Chemistry - A European Journal</i> , 2015, 21, 17100-17115. | 1.7 | 43 |
| 8627 | The HgF ₂ Ionic Switch: A Triumph of Electrostatics against Relativistic Odds. <i>Chemistry - A European Journal</i> , 2015, 21, 16848-16858. | 1.7 | 4 |
| 8628 | Unmasking the Action of Phosphinous Acid Ligands in Nitrile Hydration Reactions Catalyzed by Arene-Ruthenium(II) Complexes. <i>Chemistry - A European Journal</i> , 2015, 21, 16874-16886. | 1.7 | 42 |
| 8629 | Mechanisms of Oxygen Atom Transfer between Main-Group Elements. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 4138-4144. | 1.0 | 2 |
| 8630 | Isomer Dependence of Efficiency and Charge Recombination in Dye-Sensitized Solar Cells Using Ru Complex Dyes Bearing Halogen Substituents. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 4878-4884. | 1.0 | 7 |
| 8631 | Photoinduced Formation of an Azobenzene-Based CD-Active Supramolecular Cyclic Dimer. <i>Chemistry - A European Journal</i> , 2015, 21, 6747-6755. | 1.7 | 12 |
| 8632 | Mapping the Interactions of I ₂ , I ⁺ , I ⁺ , and I ⁺ + with Alkynes and Their Roles in Iodocyclizations. <i>Chemistry - A European Journal</i> , 2015, 21, 10191-10199. | 1.7 | 24 |
| 8633 | Long-Range π -Conjugation in Phenothiazine-containing Donor-Acceptor Dyes for Application in Dye-Sensitized Solar Cells. <i>ChemSusChem</i> , 2015, 8, 3859-3868. | 3.6 | 21 |
| 8634 | Synthesis, Structure and Redox Properties of Asymmetric (Cyclopentadienyl)(ene-1,2-dithiolate)cobalt(III) Complexes Containing Phenyl, Pyridyl and Pyrazinyl Units. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 3550-3561. | 1.0 | 10 |
| 8635 | Seven-Coordinate Luminophores: Brilliant Luminescence of Lanthanide Complexes with C_3v Geometrical Structures. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 4769-4774. | 1.0 | 60 |
| 8636 | Ein praktikables räumliches Maß für Effekte statischer Elektronenkorrelation und deren Visualisierung. <i>Angewandte Chemie</i> , 2015, 127, 12483-12488. | 1.6 | 24 |
| 8637 | Towards a better control of the radical functionalization of poly(lactic acid). <i>Polymer International</i> , 2015, 64, 631-640. | 1.6 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8638 | Poly((2-alkylbenzo[1,2,3]triazole-4,7-diyl)vinylene)s for organic solar cells. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2015, 53, 1539-1545. | 2.4 | 5 |
| 8639 | Reflectance anisotropy spectroscopy of clean and Sb covered Ge(001) surfaces and comparison with clean Si(001) surfaces. <i>Physica Status Solidi (B): Basic Research</i> , 2015, 252, 78-86. | 0.7 | 6 |
| 8640 | Gas-phase conformations of capistrucin – comparison of lasso, branched cyclic and linear topologies. <i>Rapid Communications in Mass Spectrometry</i> , 2015, 29, 1411-1419. | 0.7 | 11 |
| 8641 | Rupturing C60 Molecules into Graphene-Oxide-like Quantum Dots: Structure, Photoluminescence, and Catalytic Application. <i>Small</i> , 2015, 11, 5296-5304. | 5.2 | 39 |
| 8642 | Photoisomerization of <i>cis</i> -1,2-di(1-methyl-2-naphthyl)ethene at 77 K in Glassy Media. <i>Photochemistry and Photobiology</i> , 2015, 91, 607-615. | 1.3 | 8 |
| 8643 | Computational Investigations about the Ground and Excited States of Properties of Trans-4-N,N-Dimethylamino-4'-nitro-Stilbene (DNS) and Trans-4-N,N-Dimethyl-Amino-4'-Cyanostilbene (DCS) Derivatives. <i>Journal of Theoretical and Computational Science</i> , 2015, 02, . | 0.1 | 0 |
| 8644 | Interaction of Iron II Complexes with B-DNA. Insights from Molecular Modeling, Spectroscopy, and Cellular Biology. <i>Frontiers in Chemistry</i> , 2015, 3, 67. | 1.8 | 9 |
| 8645 | Turning-On of Coumarin Phosphorescence in Acetylacetonato Platinum Complexes of Cyclometalated Pyridyl-Substituted Coumarins. <i>Inorganics</i> , 2015, 3, 55-81. | 1.2 | 14 |
| 8646 | Water Oxidation by Ru-Polyoxometalate Catalysts: Overpotential Dependency on the Number and Charge of the Metal Centers. <i>Inorganics</i> , 2015, 3, 374-387. | 1.2 | 8 |
| 8647 | Assessing Covalency in Cerium and Uranium Hexachlorides: A Correlated Wavefunction and Density Functional Theory Study. <i>Inorganics</i> , 2015, 3, 482-499. | 1.2 | 33 |
| 8648 | Visual and Computational Comparison of Functionals Used in Density Functional Theory. <i>Mathematical and Computational Applications</i> , 2015, 20, 111-120. | 0.7 | 0 |
| 8649 | Synthesis and Antioxidant Activity of Polyhydroxylated trans-Restricted 2-Arylcinnamic Acids. <i>Molecules</i> , 2015, 20, 2555-2575. | 1.7 | 10 |
| 8650 | Mechanisms of recognition and binding of β -TTP to the plasma membrane by multi-scale molecular dynamics simulations. <i>Frontiers in Molecular Biosciences</i> , 2015, 2, 36. | 1.6 | 10 |
| 8651 | Conformational Dynamics and Binding Free Energies of Inhibitors of BACE-1: From the Perspective of Protonation Equilibria. <i>PLoS Computational Biology</i> , 2015, 11, e1004341. | 1.5 | 31 |
| 8652 | A comprehensive study of olefin metathesis catalyzed by Ru-based catalysts. <i>Beilstein Journal of Organic Chemistry</i> , 2015, 11, 1767-1780. | 1.3 | 26 |
| 8653 | Computational Modeling and Theoretical Calculations on the Interactions between Spermidine and Functional Monomer (Methacrylic Acid) in a Molecularly Imprinted Polymer. <i>Journal of Chemistry</i> , 2015, 2015, 1-9. | 0.9 | 10 |
| 8655 | Extraction Properties of β -Methyloxacalix[3]arene Methyl Ether for Alkali Metal Ions. <i>Solvent Extraction Research and Development</i> , 2015, 22, 17-24. | 0.5 | 1 |
| 8656 | Dimerization of methanimine and its charged species in the atmosphere of Titan and interstellar/cometary ice analogs. <i>Astronomy and Astrophysics</i> , 2015, 584, A76. | 2.1 | 48 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8657 | Infrared spectra and chemical abundance of methyl propionate in icy astrochemical conditions. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015, 448, 1372-1377. | 1.6 | 12 |
| 8658 | Homocoupling versus reduction of radicals: an experimental and theoretical study of Ti(scp)-mediated deoxygenation of activated alcohols. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 3462-3469. | 1.5 | 26 |
| 8659 | Modeling ultrafast exciton deactivation in oligothiophenes via nonadiabatic dynamics. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7787-7799. | 1.3 | 48 |
| 8660 | Insertion, elimination and isomerisation of olefins at alkylaluminium hydride: an experimental and theoretical study. <i>Dalton Transactions</i> , 2015, 44, 15286-15296. | 1.6 | 8 |
| 8661 | Complexation of some alkali and alkaline earth metal cations by macrocyclic compounds containing four pyridine subunits – a DFT study. <i>New Journal of Chemistry</i> , 2015, 39, 6151-6162. | 1.4 | 6 |
| 8662 | The effect of the aliphatic carboxylate linkers on the electronic structures, chemical bonding and optical properties of the uranium-based metal-organic frameworks. <i>RSC Advances</i> , 2015, 5, 26735-26748. | 1.7 | 9 |
| 8663 | Interaction between CO ₂ and ionic liquids confined in the nanopores of SAPO-11. <i>RSC Advances</i> , 2015, 5, 48908-48915. | 1.7 | 11 |
| 8664 | Critical evaluation of the potential energy surface of the CH ₃ + HO ₂ reaction system. <i>Journal of Chemical Physics</i> , 2015, 142, 054308. | 1.2 | 11 |
| 8665 | Benchmarking DFT and semiempirical methods on structures and lattice energies for ten ice polymorphs. <i>Journal of Chemical Physics</i> , 2015, 142, 124104. | 1.2 | 84 |
| 8666 | On the accuracy of density functional theory and wave function methods for calculating vertical ionization energies. <i>Journal of Chemical Physics</i> , 2015, 142, 194114. | 1.2 | 44 |
| 8667 | Charge and Spin States in Schiff Base Metal Complexes with a Disiloxane Unit Exhibiting a Strong Noninnocent Ligand Character: Synthesis, Structure, Spectroelectrochemistry, and Theoretical Calculations. <i>Inorganic Chemistry</i> , 2015, 54, 5691-5706. | 1.9 | 29 |
| 8668 | Stabilizing Coordinated Radicals via Metal-Ligand Covalency: A Structural, Spectroscopic, and Theoretical Investigation of Group 9 Tris(dithiolene) Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 3660-3669. | 1.9 | 15 |
| 8669 | Revising the Role of a Dioxirane as an Intermediate in the Uncatalyzed Hydroperoxidation of Cyclohexanone in Water. <i>Journal of Organic Chemistry</i> , 2015, 80, 6425-6431. | 1.7 | 11 |
| 8670 | Kinetics and Thermodynamics of the Reaction between the OH Radical and Adenine: A Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6516-6527. | 1.1 | 21 |
| 8671 | Unraveling the Mechanism of Photoinduced Charge Transfer in Carotenoid-Porphyrin Molecular Triad. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1231-1237. | 2.1 | 48 |
| 8672 | Global Hybrids from the Semiclassical Atom Theory Satisfying the Local Density Linear Response. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 122-131. | 2.3 | 22 |
| 8673 | The Thermochemistry of Cubane 50 Years after Its Synthesis: A High-Level Theoretical Study of Cubane and Its Derivatives. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2998-3007. | 1.1 | 16 |
| 8674 | Influence of borate structure on the thermal stability of boron-containing phenolic resins: A DFT study. <i>Polymer Degradation and Stability</i> , 2015, 119, 190-197. | 2.7 | 24 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8675 | Computational studies on hypervalent iodonium(III) compounds as activated precursors for 18F radiofluorination of electron-rich arenes. <i>Computational and Theoretical Chemistry</i> , 2015, 1066, 34-46. | 1.1 | 14 |
| 8676 | A computational study of the effects of ancillary ligands on copper(II)-ethylene interaction. <i>New Journal of Chemistry</i> , 2015, 39, 5410-5419. | 1.4 | 12 |
| 8677 | Electric properties of the low-lying excited states of benzonitrile: geometry relaxation and solvent effects. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1. | 0.5 | 13 |
| 8678 | Quantifying solvated electrons' delocalization. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 18305-18317. | 1.3 | 22 |
| 8679 | Role of exchange and correlation in the real external prediction of mutagenicity: performance of hybrid and meta-hybrid exchange-correlation functionals. <i>RSC Advances</i> , 2015, 5, 29238-29251. | 1.7 | 17 |
| 8680 | Coumarin dye with ethynyl group as π -spacer unit for dye sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2015, 310, 1-8. | 2.0 | 11 |
| 8681 | Naphthalene diimides as selective naked-eye chemosensor for copper(II) in aqueous solution. <i>Sensors and Actuators B: Chemical</i> , 2015, 212, 137-144. | 4.0 | 19 |
| 8682 | The influence of zinc(II) on thioredoxin/glutathione disulfide exchange: QM/MM studies to explore how zinc(II) accelerates exchange in higher dielectric environments. <i>Metallomics</i> , 2015, 7, 1265-1273. | 1.0 | 3 |
| 8683 | Assessment of hybrid, meta-hybrid-GGA, and long-range corrected density functionals for the estimation of enthalpies of formation, barrier heights, and ionisation potentials of selected C1-C5 oxygenates. <i>Molecular Physics</i> , 2015, 113, 1630-1635. | 0.8 | 8 |
| 8684 | B800-B850 coherence correlates with energy transfer rates in the LH2 complex of photosynthetic purple bacteria. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30805-30816. | 1.3 | 12 |
| 8685 | Toward New Solvents for EDLCs: From Computational Screening to Electrochemical Validation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 13413-13424. | 1.5 | 66 |
| 8686 | Synthesis, Solid-State Structures, and Computational Studies of Half-Sandwich Cp*BeX (X = Cl, Br, I) Compounds. <i>Organometallics</i> , 2015, 34, 3072-3078. | 1.1 | 27 |
| 8687 | The presence of cobaltdibismuth triangular faces in the lowest energy deltahedral cobaltadibismaborane polyhedra: Major differences from their cobaltadiphosphaborane analogues. <i>Journal of Organometallic Chemistry</i> , 2015, 798, 252-256. | 0.8 | 1 |
| 8688 | Piperidine-mediated annulation of 2-acylphenols with 4-nitrobenzaldehyde to 3-benzofuranones. <i>Tetrahedron Letters</i> , 2015, 56, 4175-4179. | 0.7 | 11 |
| 8689 | Anharmonic analysis of CH and OH stretching vibrations of the formic acid dimer. <i>Vibrational Spectroscopy</i> , 2015, 79, 67-75. | 1.2 | 19 |
| 8690 | Cyclometalated Zr -Selective Ruthenium Metathesis Catalysts with Modified N-Chelating Groups. <i>Organometallics</i> , 2015, 34, 2858-2869. | 1.1 | 48 |
| 8691 | Thiazolo[5,4-d]thiazole-based organic sensitizers with strong visible light absorption for transparent, efficient and stable dye-sensitized solar cells. <i>RSC Advances</i> , 2015, 5, 32657-32668. | 1.7 | 42 |
| 8692 | Quantitative Interpretation of FRET Experiments via Molecular Simulation: Force Field and Validation. <i>Biophysical Journal</i> , 2015, 108, 2721-2731. | 0.2 | 59 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8693 | A highly sensitive method for simultaneous determination of the quaternary ammonium pesticides chlormequat and mepiquat in pears and potatoes by modified QuEChERS-high performance liquid chromatography-tandem mass spectrometry. <i>RSC Advances</i> , 2015, 5, 5895-5903. | 1.7 | 10 |
| 8694 | Photophysical and photosensitizing characters of 2-phenylbenzimidazole-5-sulfonic acid. A theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 150, 187-189. | 2.0 | 4 |
| 8695 | Molecular Size and Electronic Structure Combined Effects on the Electrogenerated Chemiluminescence of Sulfurated Pyrene-Cored Dendrimers. <i>Chemistry - A European Journal</i> , 2015, 21, 2936-2947. | 1.7 | 31 |
| 8696 | Non-enzymatic Ribonucleotide Reduction in the Prebiotic Context. <i>Chemistry - A European Journal</i> , 2015, 21, 6132-6143. | 1.7 | 7 |
| 8697 | Toward assessment of density functionals for vibronic coupling in two-photon absorption: A case study of 4-nitroaniline. <i>Journal of Computational Chemistry</i> , 2015, 36, 1124-1131. | 1.5 | 12 |
| 8698 | Gas-Phase IR Spectroscopy and Structure of Biological Molecules. <i>Topics in Current Chemistry</i> , 2015, , . | 4.0 | 95 |
| 8699 | The Mechanism of E-H (E = N, O) Bond Activation by a Germanium Corrole Complex: A Combined Experimental and Computational Study. <i>Journal of the American Chemical Society</i> , 2015, 137, 7122-7127. | 6.6 | 27 |
| 8700 | Stereoselective formation and catalytic activity of hydrido(acylphosphane)(chlorido)(pyrazole)rhodium complexes. <i>Experimental and DFT studies. Dalton Transactions</i> , 2015, 44, 13141-13155. | 1.6 | 22 |
| 8701 | Reactivity Modes of an Iron Bis(alkoxide) Complex with Aryl Azides: Catalytic Nitrene Coupling vs Formation of Iron(III) Imido Dimers. <i>Organometallics</i> , 2015, 34, 2917-2923. | 1.1 | 43 |
| 8702 | Structure, stability, and aromaticity of 2,4,6,1,3,5-trisilatriphospha-benzene versus 2,4,6-trisilatriazine: A quantum chemical approach. <i>Computational and Theoretical Chemistry</i> , 2015, 1065, 18-26. | 1.1 | 3 |
| 8703 | The quest for energy traps in the CP43 antenna of photosystem II. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2015, 152, 286-300. | 1.7 | 21 |
| 8704 | A comparison of excited state properties between two different N-heterocyclic platinum(II) complexes. <i>Journal of Molecular Structure</i> , 2015, 1097, 23-28. | 1.8 | 3 |
| 8705 | The new Schiff base 4-[(4-Hydroxy-3-fluoro-5-methoxy-benzylidene)amino]-1,5-dimethyl-2-phenyl-1,2-dihydro-pyrazol-3-one: Experimental, DFT calculational studies and in vitro antimicrobial activity. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 139, 356-366. | 2.0 | 26 |
| 8706 | Theoretical study of the C-H/O-H stretching vibrations in malonaldehyde. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 145, 384-393. | 2.0 | 25 |
| 8707 | A DFT and ab initio study of conjugated and semi-conjugated mesoionic rings and their covalent isomers. <i>Tetrahedron</i> , 2015, 71, 7191-7198. | 1.0 | 30 |
| 8708 | Components of the Bond Energy in Polar Diatomic Molecules, Radicals, and Ions Formed by Group-1 and Group-2 Metal Atoms. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2968-2983. | 2.3 | 30 |
| 8709 | Improved selectivity for Pb by sulfur, selenium and tellurium analogues of 1,8-anthraquinone-18-crown-5: synthesis, spectroscopy, X-ray crystallography and computational studies. <i>Dalton Transactions</i> , 2015, 44, 11774-11787. | 1.6 | 20 |
| 8710 | Influence of Electron-Withdrawing Substituents on the Electronic Structure of Oxidized Ni and Cu Salen Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 5970-5980. | 1.9 | 71 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8711 | The origin dependence of the material constants: the permittivity and the inverse permeability. <i>Molecular Physics</i> , 2015, 113, 1899-1913. | 0.8 | 7 |
| 8712 | The 11.2 μ m emission of PAHs in astrophysical objects. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015, 448, 2960-2970. | 1.6 | 25 |
| 8713 | Capture and Release of CO ₂ in Monoethanolamine Aqueous Solutions: New Insights from First-Principles Reaction Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3189-3198. | 2.3 | 55 |
| 8714 | The infrared spectra of nonplanar polycyclic aromatic hydrocarbons with five- or seven-membered rings. <i>Chemical Physics</i> , 2015, 448, 43-52. | 0.9 | 10 |
| 8715 | Tuning the optoelectronic properties of core-substituted naphthalene diimides by the selective conversion of imides to monothioimides. <i>RSC Advances</i> , 2015, 5, 46534-46539. | 1.7 | 25 |
| 8716 | Role of Spin States in Nitric Oxide Binding to Cobalt(II) and Manganese(II) Porphyrins. Is Tighter Binding Always Stronger?. <i>Inorganic Chemistry</i> , 2015, 54, 5634-5645. | 1.9 | 24 |
| 8717 | Free electrons and ionic liquids: study of excited states by means of electron-energy loss spectroscopy and the density functional theory multireference configuration interaction method. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 15771-15780. | 1.3 | 14 |
| 8718 | Novel benzimidazole salts for lithium ion battery electrolytes: effects of substituents. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 16462-16468. | 1.3 | 6 |
| 8719 | Can acyclic conformational control be achieved via a sulfur α -fluorine gauche effect?. <i>Chemical Science</i> , 2015, 6, 3565-3571. | 3.7 | 26 |
| 8720 | Raman, infrared and NMR spectral analysis, normal coordinate analysis and theoretical calculations of 5-(methylthio)-1,3,4-thiadiazole-2(3H)-thione and its thiol tautomer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 150, 339-349. | 2.0 | 16 |
| 8721 | NMR spectroscopy studies of electronic effects and equilibrium in the organogold-to-boron transmetalation reaction and studies towards its application to the alkoxyboration addition of boron α -oxygen σ bonds to alkynes. <i>Tetrahedron</i> , 2015, 71, 4445-4449. | 1.0 | 16 |
| 8722 | Converging nuclear magnetic shielding calculations with respect to basis and system size in protein systems. <i>Journal of Biomolecular NMR</i> , 2015, 62, 327-340. | 1.6 | 47 |
| 8723 | Ionic binuclear ferrocenyl compounds containing 1,1,3,3-tetracyanopropenide anions α synthesis, structural characterization and catalytic effects on thermal decomposition of main components of solid propellants. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2015, 70, 317-326. | 0.3 | 3 |
| 8724 | On the Reaction Mechanism of the Rhodium-Catalyzed Arylation of Fullerene (C ₆₀) with Organoboron Compounds in the Presence of Water. <i>ChemistryOpen</i> , 2015, 4, 774-778. | 0.9 | 12 |
| 8725 | Conformational gating of DNA conductance. <i>Nature Communications</i> , 2015, 6, 8870. | 5.8 | 75 |
| 8726 | Magnetic Couplings in the Chemical Shift of Paramagnetic NMR. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4840-4849. | 2.3 | 69 |
| 8727 | Frozen-Density Embedding Potentials and Chiroptical Properties. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5305-5315. | 2.3 | 16 |
| 8728 | The antiradical activity of some selected flavones and flavonols. Experimental and quantum mechanical study. <i>Journal of Molecular Modeling</i> , 2015, 21, 307. | 0.8 | 56 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8729 | Identification of vibrational excitations and optical transitions of the organic electron donor tetraphenyldibenzoperiflanthene (DBP). <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30404-30416. | 1.3 | 16 |
| 8730 | Assessment of density functional methods for exciton binding energies and related optoelectronic properties. <i>RSC Advances</i> , 2015, 5, 101370-101376. | 1.7 | 47 |
| 8731 | Effects of conformational symmetry in conjugated side chains on intermolecular packing of conjugated polymers and photovoltaic properties. <i>RSC Advances</i> , 2015, 5, 106044-106052. | 1.7 | 11 |
| 8732 | Energy Alignment of Frontier Orbitals and Suppression of Charge Recombinations in P3HT/SWNT. <i>Journal of Physical Chemistry C</i> , 2015, 119, 26258-26265. | 1.5 | 7 |
| 8733 | Formation of resonantly stabilised free radicals via the reactions of atomic carbon, dicarbon, and tricarbon with unsaturated hydrocarbons: theory and crossed molecular beams experiments. <i>International Reviews in Physical Chemistry</i> , 2015, 34, 461-514. | 0.9 | 40 |
| 8734 | Organotin(IV) complexes with 5-aminoisophthalic acid: Synthesis, characterization, theoretical study, and biological activities. <i>Russian Journal of General Chemistry</i> , 2015, 85, 2386-2394. | 0.3 | 5 |
| 8735 | Four-Component Relativistic Density Functional Theory Calculations of EPR- and Hyperfine-Coupling Tensors Using Hybrid Functionals: Validation on Transition-Metal Complexes with Large Tensor Anisotropies and Higher-Order Spin-Orbit Effects. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12892-12905. | 1.1 | 49 |
| 8736 | Rational modifications on ruthenium terpyridine sensitizers with large J_{sc} for dye-sensitized solar cells: combined DFT and relativistic TDDFT studies. <i>RSC Advances</i> , 2015, 5, 100169-100175. | 1.7 | 2 |
| 8737 | Fluorescent Biotin Analogues for Microstructure Patterning and Selective Protein Immobilization. <i>Langmuir</i> , 2015, 31, 12573-12578. | 1.6 | 2 |
| 8738 | Molecular-shape selectivity by naphthalimido-modified silica stationary phases: Insight into the substituents effect of naphthalene on shape recognition and π - π interactions via electrostatic potential. <i>Journal of Chromatography A</i> , 2015, 1425, 173-179. | 1.8 | 13 |
| 8739 | New eudesmane sesquiterpenes from the marine-derived fungus <i>Penicillium thomii</i> . <i>Phytochemistry Letters</i> , 2015, 14, 209-214. | 0.6 | 18 |
| 8740 | Insights into the Spin-State Transitions in $[\text{Fe}(\text{tpy})_2]^{2+}$: Importance of the Terpyridine Rocking Motion. <i>Inorganic Chemistry</i> , 2015, 54, 11259-11268. | 1.9 | 47 |
| 8741 | The Particle-Hole Map: A Computational Tool To Visualize Electronic Excitations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5838-5852. | 2.3 | 28 |
| 8742 | Cyclopentadienide Ligand Cp^* Possessing Intrinsic Helical Chirality and Its Ferrocene Analogues. <i>Organometallics</i> , 2015, 34, 5374-5382. | 1.1 | 12 |
| 8743 | Dibenzonaphthyridinones: Heterocycle-to-Heterocycle Synthetic Strategies and Photophysical Studies. <i>Organic Letters</i> , 2015, 17, 5732-5735. | 2.4 | 10 |
| 8744 | Anthanthrene dye-sensitized solar cells: influence of the number of anchoring groups and substitution motif. <i>RSC Advances</i> , 2015, 5, 98643-98652. | 1.7 | 14 |
| 8745 | Electronically Excited States of Anisotropically Extended Singly-Deprotonated PAH Anions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 13048-13054. | 1.1 | 13 |
| 8746 | Discovery of low energy pathways to metal-mediated $\text{B}\ddot{\text{N}}$ bond reduction guided by computation and experiment. <i>Chemical Science</i> , 2015, 6, 7258-7266. | 3.7 | 6 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8747 | A (pentafluoroethyl)(trifluoromethyl)carbene complex of iridium and reductive activation of its sp ³ carbon-fluorine bonds to give perfluoro-2-butyne, perfluoro-1,2,3-butatriene | 1.6 | 9 |
| 8748 | Accelerated materials property predictions and design using motif-based fingerprints. <i>Physical Review B</i> , 2015, 92, . | 1.1 | 136 |
| 8749 | Combined Experimental and Theoretical Study on the Formation of the Elusive 2-Methyl-1-silacycloprop-2-enylidene Molecule under Single Collision Conditions via Reactions of the Silylidyne Radical (SiH; X ²) with Allene (H ₂ CCCH ₂); Tj ETQq0 0 0 rgBT /Overclock 10 Tf450 657 T | 1.1 | 12 |
| 8750 | Quadratic Corrections to Harmonic Vibrational Frequencies Outperform Linear Models. <i>Journal of Physical Chemistry A</i> , 2015, 119, 13107-13112. | 1.1 | 12 |
| 8751 | Ion pairing in ionic liquids. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 463002. | 0.7 | 108 |
| 8752 | Measurement and prediction of the NEXAFS spectra of pyrimidine and purine and the dissociation following the core excitation. <i>Chemical Physics Letters</i> , 2015, 636, 146-153. | 1.2 | 22 |
| 8753 | Singlet-Triplet Gaps of Cobalt Nitrosyls: Insights from Tropocoronand Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 7362-7367. | 1.9 | 13 |
| 8754 | Mechanistic insights into hydrogen generation for catalytic hydrolysis and alcoholysis of silanes with high-valent oxorhenium(=O) complexes. <i>Catalysis Science and Technology</i> , 2015, 5, 2157-2166. | 2.1 | 14 |
| 8755 | Physico-chemical and theoretical investigation of the Schiff's base of 2,6-diformyl-4-tert-butylphenol and m-aminocinnamic acid. <i>Russian Journal of General Chemistry</i> , 2015, 85, 2560-2567. | 0.3 | 2 |
| 8756 | Electrochemistry of Triphenylarsine-substituted Tungsten(0) Fischer carbene complexes. <i>Electrochimica Acta</i> , 2015, 186, 321-327. | 2.6 | 6 |
| 8757 | Tuning the Electronic Structure of Fe(II) Polypyridines via Donor Atom and Ligand Scaffold Modifications: A Computational Study. <i>Inorganic Chemistry</i> , 2015, 54, 8786-8793. | 1.9 | 61 |
| 8758 | The electronic configurations of LnX (Ln=La-Eu, X=O, S, Se, Te): A FON-DFT investigation. <i>Computational and Theoretical Chemistry</i> , 2015, 1068, 81-87. | 1.1 | 11 |
| 8759 | Investigating Interfacial Electron Transfer in Highly Efficient Porphyrin-Sensitized Solar Cells. <i>ACS Symposium Series</i> , 2015, , 169-188. | 0.5 | 0 |
| 8760 | Reactivity of 1,3-ynone in transformation of Ru ₂ -Ru ₄ clusters: Formation of ruthenoles via tetraruthenium intermediate. <i>Journal of Organometallic Chemistry</i> , 2015, 799-800, 166-172. | 0.8 | 10 |
| 8761 | Biacetyl monooxime ferrocenoylhydrazone and its complexing properties. <i>Russian Journal of General Chemistry</i> , 2015, 85, 2759-2764. | 0.3 | 0 |
| 8762 | Density functional investigations on the catalytic cycle of the hydrogenation of aldehydes catalyzed by an enhanced ruthenium complex: an alcohol-bridged autocatalytic process. <i>RSC Advances</i> , 2015, 5, 2827-2836. | 1.7 | 1 |
| 8763 | Assessing density functionals for the prediction of thermochemistry of Ti-O-Cl species. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550055. | 1.8 | 2 |
| 8764 | Bond Dissociation Energy of Halogen Oxides. <i>Procedia Chemistry</i> , 2015, 17, 99-105. | 0.7 | 2 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8765 | Current limitations of molecular dynamic simulations as probes of thermo-physical behavior of silicate melts. <i>American Mineralogist</i> , 2015, 100, 1866-1882. | 0.9 | 14 |
| 8766 | Ab Initio Simulations and Electronic Structure of Lithium-Doped Ionic Liquids: Structure, Transport, and Electrochemical Stability. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14705-14719. | 1.2 | 49 |
| 8767 | The competition between H ₂ O and CO ₂ adhesion at reservoir conditions: A DFT study of simple mineral models and the entropy, ZPE, dispersion and T, P variations. <i>Computational and Theoretical Chemistry</i> , 2015, 1073, 55-60. | 1.1 | 5 |
| 8768 | Role of Water in the Puzzling Mechanism of the Final Aromatization Step Promoted by the Human Aromatase Enzyme. Insights from QM/MM MD Simulations. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2218-2226. | 2.5 | 25 |
| 8769 | Oxovanadium(IV) Schiff Base Complex Derived From Phenylalanine Analogue Containing 2,3-Diaminopropionic Acid (DAP): Synthesis, Computational Study, and Biological Evaluation. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 2015, 45, 455-467. | 0.6 | 2 |
| 8770 | Labile Capping Bonds in Lanthanide(III) Complexes: Shorter and Weaker. <i>Journal of Physical Chemistry A</i> , 2015, 119, 774-780. | 1.1 | 17 |
| 8771 | Impact of sulfur heteroatoms on the activity of quaternary ammonium salts as phase transfer catalysts for nucleophilic displacement reactions. <i>Journal of Molecular Catalysis A</i> , 2015, 398, 282-288. | 4.8 | 3 |
| 8772 | A Nickel Phosphine Complex as a Fast and Efficient Hydrogen Production Catalyst. <i>Journal of the American Chemical Society</i> , 2015, 137, 1109-1115. | 6.6 | 137 |
| 8773 | Theoretical studies on the electronic structure and spectroscopic properties of zinc(II) bis(dipyrrinate)s. <i>Computational and Theoretical Chemistry</i> , 2015, 1054, 88-92. | 1.1 | 14 |
| 8774 | Performances of DFT methods implemented in G09 for simulations of the dispersion-dominated CH ₃ protein complex: A case study with glycerol-GDH. <i>Journal of Molecular Structure</i> , 2015, 1084, 223-228. | 1.8 | 11 |
| 8775 | TEMPO-mediated homocoupling of aryl Grignard reagents: mechanistic studies. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 2762-2767. | 1.5 | 21 |
| 8776 | Homopolymerization of Ethylene by Palladium Phosphine Sulfonate Catalysts: The Role of Structural and Environmental Factors. <i>Organometallics</i> , 2015, 34, 373-380. | 1.1 | 8 |
| 8777 | Photophysics, photochemistry and thermal stability of diarylethene-containing benzothiazolium species. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2015, 301, 20-31. | 2.0 | 5 |
| 8778 | Computational design and development of a novel voltammetric sensor for minoxidil detection based on electropolymerized molecularly imprinted polymer. <i>Journal of Electroanalytical Chemistry</i> , 2015, 740, 45-52. | 1.9 | 43 |
| 8779 | Theoretical studies of Raman scattering properties of methylphosphine and methylamine adsorbed on gold clusters. <i>Vibrational Spectroscopy</i> , 2015, 76, 38-47. | 1.2 | 5 |
| 8780 | Vibrational Circular Dichroism Absolute Configuration Determination of Natural Products. <i>Progress in the Chemistry of Organic Natural Products</i> , 2015, 100, 311-452. | 0.8 | 59 |
| 8781 | Structural, vibrational and thermodynamic properties of Mg and Mg_2 and Mg_3 . <i>Physics of the Earth and Planetary Interiors</i> , 2015, 240, 1-24. | 0.7 | 30 |
| 8782 | Mechanistic Investigation Into Catalytic Hydrosilylation with a High-Valent Ruthenium(VI) Nitrido Complex: A DFT Study. <i>Organometallics</i> , 2015, 34, 212-220. | 1.1 | 13 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 8783 | The spectroscopic (FT-IR, UV-vis), Fukui function, NLO, NBO, NPA and tautomerism effect analysis of (E)-2-[(2-hydroxy-6-methoxybenzylidene)amino]benzoxonitrile. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 139, 539-548. | 2.0 | 87 |
| 8784 | Ferrocenoylhydrazone of 2-N-tosylaminobenzaldehyde: Structure, properties, and complexing ability. <i>Russian Journal of General Chemistry</i> , 2015, 85, 126-134. | 0.3 | 2 |
| 8785 | A QM/MM study of the initial steps of catalytic mechanism of nitrile hydratase. <i>Chemical Physics Letters</i> , 2015, 623, 8-13. | 1.2 | 8 |
| 8786 | Fuels From Biomass: An Interdisciplinary Approach. <i>Notes on Numerical Fluid Mechanics and Multidisciplinary Design</i> , 2015, , . | 0.2 | 0 |
| 8787 | Azobenzene-Functionalized Cage Silsesquioxanes as Inorganic-Organic Hybrid, Photoresponsive, Nanoscale, Building Blocks. <i>Chemistry - A European Journal</i> , 2015, 21, 4731-4738. | 1.7 | 38 |
| 8788 | Simulation of X-ray absorption spectra with orthogonality constrained density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14360-14374. | 1.3 | 54 |
| 8789 | Density Functional Theory of the Water Splitting Reaction on Fe(0): Comparison of Local and Nonlocal Correlation Functionals. <i>ACS Catalysis</i> , 2015, 5, 2070-2080. | 5.5 | 28 |
| 8790 | The Association of Two Frustrated Lewis Pairs by State-of-the-Art Quantum Chemical Methods. <i>Israel Journal of Chemistry</i> , 2015, 55, 235-242. | 1.0 | 23 |
| 8791 | Theoretical study of the dimerization of aqueous beryllium cations. <i>Journal of Molecular Modeling</i> , 2015, 21, 6. | 0.8 | 18 |
| 8792 | Geometry of the magic number $H_{21}O_{21}$ water cluster by proxy. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5466-5473. | 1.3 | 9 |
| 8793 | Silica microspheres containing high density surface hydroxyl groups as efficient epoxidation catalysts. <i>RSC Advances</i> , 2015, 5, 21125-21131. | 1.7 | 11 |
| 8794 | Molecular modeling and experimental studies on structure and NMR parameters of 9-benzyl-3,6-diiodo-9H-carbazole. <i>Structural Chemistry</i> , 2015, 26, 997-1006. | 1.0 | 18 |
| 8795 | Theoretical analysis of [5.5.6]cyclacenes: electronic properties, strain energies and substituent effects. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7366-7372. | 1.3 | 27 |
| 8796 | Theoretical study on the stability of double-decker type metal phthalocyanines, $M(Pc)_2$ and $M(Pc)_2^{+}$ (M = Ti, Sn and Sc): a critical assessment on the performance of density functionals. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6478-6483. | 1.3 | 9 |
| 8797 | A single atom change switches-on the solar-to-energy conversion efficiency of Zn-porphyrin based dye sensitized solar cells to 10.5%. <i>Energy and Environmental Science</i> , 2015, 8, 1368-1375. | 15.6 | 66 |
| 8798 | Rational design of long-wavelength absorbing and emitting carbostyrils aided by time-dependent density functional calculations. <i>Computational and Theoretical Chemistry</i> , 2015, 1055, 25-32. | 1.1 | 4 |
| 8799 | Synthesis, molecular structure, spectroscopic analysis, thermodynamic parameters and molecular modeling studies of (2-methoxyphenyl)oxalate. <i>Journal of Molecular Structure</i> , 2015, 1087, 104-112. | 1.8 | 14 |
| 8800 | Structural properties of methanol-water binary mixtures within the quantum cluster equilibrium model. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8467-8479. | 1.3 | 56 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8801 | Determining the cohesive energy of coronene by dispersion-corrected DFT methods: Periodic boundary conditions vs. molecular pairs. <i>Journal of Chemical Physics</i> , 2015, 142, 054702. | 1.2 | 10 |
| 8802 | Rationalizing the photophysical properties of BODIPY laser dyes via aromaticity and electron-donor-based structural perturbations. <i>Dyes and Pigments</i> , 2015, 116, 74-81. | 2.0 | 14 |
| 8803 | Hafnium catalysts for direct alkene epoxidation using molecular oxygen as oxidant. <i>RSC Advances</i> , 2015, 5, 12311-12322. | 1.7 | 6 |
| 8804 | Multinuclear Diffusion NMR Spectroscopy and DFT Modeling: A Powerful Combination for Unraveling the Mechanism of Phosphoester Bond Hydrolysis Catalyzed by Metal-Substituted Polyoxometalates. <i>Chemistry - A European Journal</i> , 2015, 21, 4428-4439. | 1.7 | 47 |
| 8805 | Stacking of Metal Chelates with Benzene: Can Dispersion-Corrected DFT Be Used to Calculate Organic-Inorganic Stacking?. <i>ChemPhysChem</i> , 2015, 16, 761-768. | 1.0 | 14 |
| 8806 | Vibrational and electronic peculiarities of NiTiO ₃ nanostructures inferred from first principle calculations. <i>RSC Advances</i> , 2015, 5, 17396-17404. | 1.7 | 37 |
| 8807 | Assessing the Suitability of the Multilevel Strategy for the Conformational Analysis of Small Ligands. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1164-1172. | 1.2 | 16 |
| 8808 | Benchmark of electronic structure methods for protein-ligand interactions based on high-level reference data. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1540001. | 1.8 | 7 |
| 8809 | Can B3LYP be improved by optimization of the proportions of exchange and correlation functionals?. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 502-509. | 1.0 | 21 |
| 8810 | Vertical excitation energies of linear cyanine dyes by spin-flip time-dependent density functional theory. <i>Chemical Physics Letters</i> , 2015, 622, 115-119. | 1.2 | 13 |
| 8811 | Solvent effect in keto-enol tautomerism for a polymerizable β -ketonitrile monomer. <i>Spectroscopy and theoretical study. Journal of Molecular Structure</i> , 2015, 1081, 375-380. | 1.8 | 5 |
| 8812 | A computational study on high-valent mono-oxo-rhenium(V) complex-catalyzed hydrosilylation of carbonyls: What a difference an oxo ligand makes. <i>Journal of Molecular Catalysis A</i> , 2015, 400, 31-41. | 4.8 | 7 |
| 8813 | Genetic Algorithm Optimization of Point Charges in Force Field Development: Challenges and Insights. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1422-1434. | 1.1 | 24 |
| 8814 | Semi-Experimental Equilibrium Structure Determinations by Employing B3LYP/SNSD Anharmonic Force Fields: Validation and Application to Semirigid Organic Molecules. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2058-2082. | 1.1 | 155 |
| 8815 | Theoretical investigation on the mechanism and dynamics of oxo exchange of neptunyl(^{VI}) hydroxide in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7537-7547. | 1.3 | 2 |
| 8816 | Structural Characterization of Frustrated Lewis Pairs and Their Reaction Products Using Modern Solid-State NMR Spectroscopy Techniques. <i>Israel Journal of Chemistry</i> , 2015, 55, 150-178. | 1.0 | 17 |
| 8817 | Establishing the Steric Bulk of Main Group Hydrides in Reduction Reactions. <i>Israel Journal of Chemistry</i> , 2015, 55, 226-234. | 1.0 | 8 |
| 8818 | Error Accumulations in Adhesive Energies of Dihydrogen Molecular Chains: Performances of the XYG3 Type of Doubly Hybrid Density Functionals. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1590-1599. | 1.1 | 13 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8819 | Polarizable Density Embedding: A New QM/QM/MM-Based Computational Strategy. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5344-5355. | 1.1 | 78 |
| 8820 | Restricted Hartree Fock using complex-valued orbitals: A long-known but neglected tool in electronic structure theory. <i>Journal of Chemical Physics</i> , 2015, 142, 024104. | 1.2 | 26 |
| 8821 | Stereoselective Formation of Eight-Membered Rings by Radical Cyclization of Silylenedioxy-Tethered Bis-methacrylate Derivatives. <i>Journal of Organic Chemistry</i> , 2015, 80, 2869-2873. | 1.7 | 4 |
| 8822 | Resonant-Convergent PCM Response Theory for the Calculation of Second Harmonic Generation in Makaluvamines A: Pyrroloiminoquinone Marine Natural Products from Poriferans of Genus <i>Zyzya</i> . <i>Journal of Physical Chemistry A</i> , 2015, 119, 5368-5376. | 1.1 | 6 |
| 8823 | Effect of H ₂ Binding on the Nonadiabatic Transition Probability between Singlet and Triplet States of the [NiFe]-Hydrogenase Active Site. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1066-1073. | 1.1 | 21 |
| 8824 | Halide Binding and Inhibition of Laccase Copper Clusters: The Role of Reorganization Energy. <i>Inorganic Chemistry</i> , 2015, 54, 476-483. | 1.9 | 33 |
| 8825 | Quantum Chemistry Study of Proton Transport in Imidazole Chains. <i>Journal of Physical Chemistry B</i> , 2015, 119, 3213-3222. | 1.2 | 24 |
| 8826 | Prediction Uncertainty of Density Functional Approximations for Properties of Crystals with Cubic Symmetry. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5288-5304. | 1.1 | 78 |
| 8827 | High-Level QM/MM Calculations Support the Concerted Mechanism for Michael Addition and Covalent Complex Formation in Thymidylate Synthase. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 713-722. | 2.3 | 20 |
| 8828 | Theoretical Examination of the C=P Anomeric Effect. <i>Journal of Organic Chemistry</i> , 2015, 80, 2879-2883. | 1.7 | 21 |
| 8829 | Effect of Molecular-Level Insulation on the Performance of a Dye-Sensitized Solar Cell: Fluorescence Studies in Solid State. <i>Journal of Fluorescence</i> , 2015, 25, 59-68. | 1.3 | 10 |
| 8830 | Calculating High Energy Charge Transfer States Using Optimally Tuned Range-Separated Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1110-1117. | 2.3 | 51 |
| 8831 | Feasibility of Valence-to-Core X-ray Emission Spectroscopy for Tracking Transient Species. <i>Journal of Physical Chemistry C</i> , 2015, 119, 14571-14578. | 1.5 | 40 |
| 8832 | Protein Conformational Landscapes and Catalysis. Influence of Active Site Conformations in the Reaction Catalyzed by L-Lactate Dehydrogenase. <i>ACS Catalysis</i> , 2015, 5, 1172-1185. | 5.5 | 48 |
| 8833 | Benchmarking the CO ₂ Adsorption Energy on Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2015, 119, 4934-4948. | 1.5 | 47 |
| 8834 | Spin Adapted versus Broken Symmetry Approaches in the Description of Magnetic Coupling in Heterodinuclear Complexes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1006-1019. | 2.3 | 14 |
| 8835 | Steady-State and Femtosecond Transient Absorption Spectroscopy of New Two-Photon Absorbing Fluorene-Containing Quinolinium Cation Membrane Probes. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 2833-2846. | 4.0 | 32 |
| 8836 | Self-Assembly of Peptide Nanostructures onto an Electrode Surface for Nonenzymatic Oxygen Sensing. <i>Journal of Physical Chemistry C</i> , 2015, 119, 1038-1046. | 1.5 | 22 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8837 | Comparison of Real-Time and Linear-Response Time-Dependent Density Functional Theories for Molecular Chromophores Ranging from Sparse to High Densities of States. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1102-1109. | 2.3 | 98 |
| 8838 | Infrared Identification of Proton-Bound Rare-Gas Dimers (XeHXe) ⁺ , (KrHKr) ⁺ , and (KrHXe) ⁺ and Their Deuterated Species in Solid Hydrogen. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2651-2660. | 1.1 | 23 |
| 8839 | Twin Laws and Energy in Monoclinic Hydroxyapatite, Ca ₅ (PO ₄) ₃ (OH). <i>Crystal Growth and Design</i> , 2015, 15, 411-418. | 1.4 | 13 |
| 8840 | Diffusion Monte Carlo Study of <i>para</i> -Diiodobenzene Polymorphism Revisited. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 907-917. | 2.3 | 22 |
| 8841 | Reassessment of the Thermodynamic, Kinetic, and Spectroscopic Features of Cyanomethanimine Derivatives: A Full Anharmonic Perturbative Treatment. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1165-1171. | 2.3 | 19 |
| 8842 | Kinetic and mechanistic insight into Lewis base and acid-mediated phenylselenoetherification of 2,6-dimethyl-hept-5-en-2-ol. <i>Structural Chemistry</i> , 2015, 26, 915-922. | 1.0 | 6 |
| 8843 | Dissociation of 1,1,1-Trifluoroethane Is an Intrinsic RRKM Process: Classical Trajectories and Successful Master Equation Modeling. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1846-1858. | 1.1 | 14 |
| 8844 | Accurate reaction barrier heights of pericyclic reactions: Surprisingly large deviations for the CBS-QB3 composite method and their consequences in DFT benchmark studies. <i>Journal of Computational Chemistry</i> , 2015, 36, 622-632. | 1.5 | 124 |
| 8845 | Cleavage of the \hat{I}^2O_4 linkage of lignin using group 8 pincer complexes: A DFT study. <i>Journal of Molecular Catalysis A</i> , 2015, 399, 33-41. | 4.8 | 19 |
| 8846 | Bicyclobutonium Ions in Biosynthesis – Interconversion of Cyclopropyl-Containing Sterols from Orchids. <i>Journal of the American Chemical Society</i> , 2015, 137, 2085-2088. | 6.6 | 22 |
| 8847 | Calculating Electron-Transfer Coupling with Density Functional Theory: The Long-Range-Corrected Density Functionals. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7480-7490. | 1.2 | 31 |
| 8848 | Origins of Stereoselectivity in Intramolecular Aldol Reactions Catalyzed by Cinchona Amines. <i>Journal of the American Chemical Society</i> , 2015, 137, 2116-2127. | 6.6 | 74 |
| 8849 | Comparison of vibrational dynamics, thermal behaviour, and phase transition in [Ni(NH ₃) ₄](ReO ₄) ₂ and [Ni(NH ₃) ₆](ReO ₄) ₂ . <i>Journal of Thermal Analysis and Calorimetry</i> , 2015, 119, 1415-1428. | 2.0 | 13 |
| 8850 | A QM/MM study of Kempptide phosphorylation catalyzed by protein kinase A. The role of Asp166 as a general acid/base catalyst. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 3497-3511. | 1.3 | 18 |
| 8851 | Assessment of Several DFT Functionals in Calculation of the Reduction Potentials for Ni ²⁺ , Pd ²⁺ , and Pt ²⁺ Bis-ethylene-1,2-dithiolene and -Diselenolene Complexes. <i>Journal of Physical Chemistry A</i> , 2015, 119, 911-918. | 1.1 | 25 |
| 8852 | Anandamide Hydrolysis in FAAH Reveals a Dual Strategy for Efficient Enzyme-Assisted Amide Bond Cleavage via Nitrogen Inversion. <i>Journal of Physical Chemistry B</i> , 2015, 119, 789-801. | 1.2 | 36 |
| 8853 | Trichloroalane addition to bis(silyl)amino-silyliminoboranes: a theoretical study. <i>Journal of the Iranian Chemical Society</i> , 2015, 12, 183-190. | 1.2 | 0 |
| 8854 | Understanding the Hydrolysis Mechanism of Ethyl Acetate Catalyzed by an Aqueous Molybdocene: A Computational Chemistry Investigation. <i>Inorganic Chemistry</i> , 2015, 54, 1223-1231. | 1.9 | 13 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8855 | Directed Functionalization of Halophenyl-2-oxazolines with TMPMgCl·LiCl. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 967-977. | 1.2 | 21 |
| 8856 | Quantum chemical study on the inhibition efficiencies of some sym-triazines as inhibitors for mild steel in acidic medium. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2015, 50, 306-313. | 2.7 | 41 |
| 8857 | Large Scale GW Calculations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2680-2696. | 2.3 | 255 |
| 8858 | Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer in a Solvated Phenol-Amine Complex. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2758-2768. | 1.2 | 48 |
| 8859 | Spin-Vibronic Quantum Dynamics for Ultrafast Excited-State Processes. <i>Accounts of Chemical Research</i> , 2015, 48, 809-817. | 7.6 | 96 |
| 8860 | Proton or Metal? The H/D Exchange of Arenes in Acidic Solvents. <i>ACS Catalysis</i> , 2015, 5, 769-775. | 5.5 | 54 |
| 8861 | Third-order nonlinear optical properties of 3,4-ethylenedioxythiophene copolymers with chalcogenadiazole acceptors. <i>New Journal of Chemistry</i> , 2015, 39, 2795-2806. | 1.4 | 26 |
| 8862 | Tuning the optical and electrochemical properties of core-substituted naphthalenediimides with styryl imide substituent. <i>New Journal of Chemistry</i> , 2015, 39, 2506-2514. | 1.4 | 6 |
| 8863 | Enantioselective Organocatalytic Reduction of α -Trifluoromethyl Nitroalkenes: An Efficient Strategy for the Synthesis of Chiral α -Trifluoromethyl Amines. <i>Chemistry - A European Journal</i> , 2015, 21, 3589-3595. | 1.7 | 35 |
| 8864 | NLO Properties of Unidirectional Lengthening $[Pt_3(CO)_3(\mu_2-CO)_3]_n$ Clusters: A TDDFT Study. <i>Journal of Cluster Science</i> , 2015, 26, 1511-1526. | 1.7 | 0 |
| 8865 | Raman spectroscopy study of the interaction of 3,5,3'-triiodo-L-thyronine with phosphatidylglycerol lipid bilayers. <i>Journal of Raman Spectroscopy</i> , 2015, 46, 302-308. | 1.2 | 9 |
| 8866 | Three-center bonding analyzed from correlated and uncorrelated third-order reduced density matrices. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 173-179. | 1.1 | 8 |
| 8867 | Theoretical modeling of friction and wear processes at atomic level. , 2015, , 385-405. | | 4 |
| 8868 | Efficient Implementation of the Pair Atomic Resolution of the Identity Approximation for Exact Exchange for Hybrid and Range-Separated Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 518-527. | 2.3 | 46 |
| 8869 | Square-Antiprismatic Eight-Coordinate Complexes of Divalent First-Row Transition Metal Cations: A Density Functional Theory Exploration of the Electronic-Structural Landscape. <i>Inorganic Chemistry</i> , 2015, 54, 1375-1383. | 1.9 | 7 |
| 8870 | Photoisomerization of Silyl-Substituted Cyclobutadiene Induced by $\tilde{f}^* \tilde{f}^*$ Excitation: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 442-451. | 1.1 | 1 |
| 8871 | Formation of charge transfer complexes significantly improves the electron transfer process of polymer solar cells. <i>Organic Electronics</i> , 2015, 18, 70-76. | 1.4 | 5 |
| 8872 | The Synthesis and STM/AFM Imaging of β -Olympicene™ Benzo[<i>a</i>]pyrenes. <i>Chemistry - A European Journal</i> , 2015, 21, 2011-2018. | 1.7 | 39 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8873 | Semilocal density functional obeying a strongly tightened bound for exchange. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 685-689. | 3.3 | 119 |
| 8874 | Structural characterization, vibrational, optical properties and DFT investigation of a new luminescent organic-inorganic material: (C ₆ H ₁₄ N) ₃ Bi ₂ I ₉ . Journal of Luminescence, 2015, 161, 214-220. | 1.5 | 75 |
| 8875 | Tailoring of Energy Levels in D-π-A Organic Dyes via Fluorination of Acceptor Units for Efficient Dye-Sensitized Solar Cells. Scientific Reports, 2015, 5, 7711. | 1.6 | 45 |
| 8876 | Interaction of C ₆₀ with Water: First-Principles Modeling and Environmental Implications. Environmental Science & Technology, 2015, 49, 1529-1536. | 4.6 | 37 |
| 8877 | Computational Methodology Study of the Optical and Thermochemical Properties of a Molecular Photoswitch. Journal of Physical Chemistry A, 2015, 119, 896-904. | 1.1 | 57 |
| 8878 | Supramolecular Recognition Influences Magnetism in [X@HV ^{IV}] ₈ V ^V ₁₄ O ₅₄] ⁶⁺ Self-Assemblies with Symmetry-Breaking Guest Anions. Chemistry - A European Journal, 2015, 21, 2387-2397. | 1.7 | 38 |
| 8879 | Structural, thermal and quantum chemical studies of p-coumaric and caffeic acids. Journal of Molecular Structure, 2015, 1085, 242-248. | 1.8 | 39 |
| 8880 | Heteroleptic Ru(II)-terpyridine complex and its metal-containing conducting polymer: Synthesis and characterization. Synthetic Metals, 2015, 200, 109-116. | 2.1 | 5 |
| 8881 | Development of a ReaxFF Potential for Carbon Condensed Phases and Its Application to the Thermal Fragmentation of a Large Fullerene. Journal of Physical Chemistry A, 2015, 119, 571-580. | 1.1 | 243 |
| 8882 | Supertetrahedral B ₈₀ H ₂₀ , C ₈₀ H ₂₀ , and Al ₈₀ H ₂₀ analogs of dodecahedrane and their substituted molecules. Structural Chemistry, 2015, 26, 223-229. | 1.0 | 13 |
| 8883 | Attosecond Hole Migration in Benzene Molecules Surviving Nuclear Motion. Journal of Physical Chemistry Letters, 2015, 6, 426-431. | 2.1 | 105 |
| 8884 | Structural and Electronic Properties of Photoexcited TiO ₂ Nanoparticles from First Principles. Journal of Chemical Theory and Computation, 2015, 11, 635-645. | 2.3 | 32 |
| 8885 | Ab Initio Characterization of the Electrochemical Stability and Solvation Properties of Condensed-Phase Ethylene Carbonate and Dimethyl Carbonate Mixtures. Journal of Physical Chemistry C, 2015, 119, 3865-3880. | 1.5 | 50 |
| 8886 | Co(III) complexes of tetradentate X ₃ L type ligands: Synthesis, electronic structure, and reactivity. Inorganica Chimica Acta, 2015, 430, 30-35. | 1.2 | 11 |
| 8887 | Design of novel tetra-hetero[8]circulenes: a theoretical study of electronic structure and charge transport characteristics. RSC Advances, 2015, 5, 24167-24174. | 1.7 | 13 |
| 8888 | Second-Generation Fluorescent Quadracyclic Adenine Analogues: Environment-Responsive Probes with Enhanced Brightness. Chemistry - A European Journal, 2015, 21, 4039-4048. | 1.7 | 22 |
| 8889 | Structural and electronic properties of sodium clusters under confinement. Physical Review B, 2015, 91, . | 1.1 | 2 |
| 8890 | Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. Computer Physics Communications, 2015, 192, 60-69. | 3.0 | 133 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8891 | Heteroleptic platinum(κ^2) NHC complexes with a C^*C^* cyclometalated ligand – synthesis, structure and photophysics. <i>Journal of Materials Chemistry C</i> , 2015, 3, 1680-1693. | 2.7 | 55 |
| 8892 | Stabilizing non-covalent interactions of ligand aromatic moieties and proline in ligand–protein systems. <i>Monatshefte für Chemie</i> , 2015, 146, 389-397. | 0.9 | 4 |
| 8893 | Protolytic and complexation properties of the cyclic thiosemicarbazone ligand. <i>Russian Journal of General Chemistry</i> , 2015, 85, 92-96. | 0.3 | 5 |
| 8894 | Modeling the antiferromagnetic MnII/MnII system within the protein phosphatase-5 catalytic site. <i>Journal of Molecular Modeling</i> , 2015, 21, 14. | 0.8 | 5 |
| 8895 | Rearrangement of Metallabenzynes to Chlorocyclopentadienyl Complexes. <i>Organometallics</i> , 2015, 34, 890-896. | 1.1 | 29 |
| 8896 | Mechanism of the reactions of ruthenium(II) polypyridyl complexes with thiourea, sulfur-containing amino acids and nitrogen-containing heterocycles. <i>Polyhedron</i> , 2015, 91, 73-83. | 1.0 | 19 |
| 8897 | Tuning electronic and magnetic properties of GaN nanosheets by surface modifications and nanosheet thickness. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8692-8698. | 1.3 | 26 |
| 8898 | Enantiomeric discrimination of chiral organic salts by chiral aza-15-crown-5 ether with C_1 symmetry: experimental and theoretical approaches. <i>Journal of Molecular Modeling</i> , 2015, 21, 55. | 0.8 | 7 |
| 8899 | Preparation of candidate reference materials for the determination of phosphorus containing flame retardants in styrene-based polymers. <i>Analytical and Bioanalytical Chemistry</i> , 2015, 407, 3023-3034. | 1.9 | 4 |
| 8900 | Computational and spectroscopic characterization of key intermediates of the Selective Catalytic Reduction cycle of NO on zeolite-supported Cu catalyst. <i>Inorganica Chimica Acta</i> , 2015, 430, 132-143. | 1.2 | 16 |
| 8901 | Synthesis, spectral analysis, structural elucidation and quantum chemical studies of (E)-methyl-4-[(2-phenylhydrazono)methyl]benzoate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 143, 91-100. | 2.0 | 21 |
| 8902 | An analysis of hydrated proton diffusion in <i>ab initio</i> molecular dynamics. <i>Journal of Chemical Physics</i> , 2015, 142, 014104. | 1.2 | 63 |
| 8903 | A Case Study of the Mechanism of Alcohol-Mediated Morita Baylis–Hillman Reactions. The Importance of Experimental Observations. <i>Journal of the American Chemical Society</i> , 2015, 137, 3811-3826. | 6.6 | 368 |
| 8904 | Calculated Nuclear Magnetic Resonance Spectra of Polytwistane and Related Hydrocarbon Nanorods. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1020-1026. | 2.3 | 7 |
| 8905 | Synthesis and structure of 1-benzyl-5-amino-1H-tetrazole in the solid state and in solution: Combining X-ray diffraction, 1H NMR, FT–IR, and UV–Vis spectra and DFT calculations. <i>Comptes Rendus Chimie</i> , 2015, 18, 422-429. | 0.2 | 13 |
| 8906 | A Fine Line Separates Carbocations from Diradical Ions in Donor-Unconjugated Cations. <i>Journal of the American Chemical Society</i> , 2015, 137, 3402-3410. | 6.6 | 26 |
| 8907 | N-Trinitroethyl-substituted azoxyfurazan: high detonation performance energetic materials. <i>RSC Advances</i> , 2015, 5, 27305-27312. | 1.7 | 26 |
| 8908 | Imino-N-Heterocyclic Carbene Palladium(II) Complex-Catalyzed Direct Arylation of Electron-Deficient Fluoroarenes with α -On and Off–Chelating Effect Assistance. <i>Organometallics</i> , 2015, 34, 1021-1028. | 1.1 | 13 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 8909 | Two-Dimensionally Extended π -Conjugation of Donor-Acceptor Copolymers via Oligothieryl Side Chains for Efficient Polymer Solar Cells. <i>Macromolecules</i> , 2015, 48, 1723-1735. | 2.2 | 69 |
| 8910 | Theoretical investigations of the perylene electronic structure: Monomer, dimers, and excimers. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 442-452. | 1.0 | 57 |
| 8911 | Charge Separation Dynamics and Optoelectronic Properties of a Diaminoterephthalate- β -Cyanoethyl Diad. <i>Advanced Functional Materials</i> , 2015, 25, 2047-2053. | 7.8 | 16 |
| 8912 | Photoswitching Behavior of a Cyclohexene-Bridged versus a Cyclopentene-Bridged Dithienylethene System. <i>ChemPhysChem</i> , 2015, 16, 1491-1501. | 1.0 | 8 |
| 8913 | Self-consistent continuum solvation for optical absorption of complex molecular systems in solution. <i>Journal of Chemical Physics</i> , 2015, 142, 034111. | 1.2 | 17 |
| 8914 | Binding of bivalent metal cations by α -D-Glucuronate: insights from the DFT-MD simulations. <i>New Journal of Chemistry</i> , 2015, 39, 3987-3994. | 1.4 | 19 |
| 8915 | Benchmark thermodynamic properties of methylanisoles: Experimental and theoretical study. <i>Journal of Chemical Thermodynamics</i> , 2015, 85, 155-162. | 1.0 | 54 |
| 8916 | Pyridine-triazole ligands for copper-catalyzed aerobic alcohol oxidation. <i>RSC Advances</i> , 2015, 5, 55847-55855. | 1.7 | 23 |
| 8917 | Dispersion- and Exchange-Corrected Density Functional Theory for Sodium Ion Hydration. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2958-2967. | 2.3 | 42 |
| 8918 | Suppressing of slow magnetic relaxation in tetracoordinate Co(II) field-induced single-molecule magnet in hybrid material with ferromagnetic barium ferrite. <i>Scientific Reports</i> , 2015, 5, 10761. | 1.6 | 25 |
| 8919 | DFT study on addition reaction mechanism of guanine-cytosine base pair with OH radical. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 437-444. | 0.9 | 10 |
| 8920 | Structural evolution of nucleobase clusters using force field models and density functional theory. <i>Chemical Physics Letters</i> , 2015, 634, 166-173. | 1.2 | 2 |
| 8921 | Establishing the Catalytic Mechanism of Human Pancreatic α -Amylase with QM/MM Methods. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2508-2516. | 2.3 | 32 |
| 8922 | Can Multiconfigurational Self-Consistent Field Theory and Density Functional Theory Correctly Predict the Ground State of Metal-Metal-Bonded Complexes?. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4093-4101. | 2.3 | 20 |
| 8923 | Reaction barrier heights for cycloreversion of heterocyclic rings: An Achilles' heel for DFT and standard ab initio procedures. <i>Chemical Physics</i> , 2015, 458, 1-8. | 0.9 | 68 |
| 8924 | A theoretical investigation of the atmospherically important reaction between chlorine atoms and formic acid: determination of the reaction mechanism and calculation of the rate coefficient at different temperatures. <i>Molecular Physics</i> , 2015, 113, 1511-1533. | 0.8 | 8 |
| 8925 | Toward a Unified Mechanism for Oxoammonium Salt-Mediated Oxidation Reactions: A Theoretical and Experimental Study Using a Hydride Transfer Model. <i>Journal of Organic Chemistry</i> , 2015, 80, 8150-8167. | 1.7 | 55 |
| 8926 | Stability and Vibrations of Guest Molecules in the Type II Clathrate Hydrate: A First-Principles Study of Solid Phase. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7063-7069. | 1.1 | 19 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8927 | Theoretical studies of organotin(IV) complexes derived from ONO-donor type schiff base ligands. <i>Journal of Molecular Modeling</i> , 2015, 21, 221. | 0.8 | 14 |
| 8928 | Stability, Reactivity, Selectivity, Catalysis, and Predictions of 1,3,2,5-Diazadiborinine: Computational Insight into a Boron-Boron Frustrated Lewis Pair. <i>Journal of Organic Chemistry</i> , 2015, 80, 8790-8795. | 1.7 | 24 |
| 8929 | Synthesis of some new 5-substituted-3-phenyl-4-thioxo-2-thiazolidinones and their fused thiopyrano[2,3-d]thiazole derivatives. <i>Journal of Sulfur Chemistry</i> , 2015, 36, 511-525. | 1.0 | 4 |
| 8930 | Factors affecting the solubility of ionic compounds. <i>Computational and Theoretical Chemistry</i> , 2015, 1069, 132-137. | 1.1 | 10 |
| 8931 | Choosing a density functional for static molecular polarizabilities. <i>Chemical Physics Letters</i> , 2015, 635, 257-261. | 1.2 | 39 |
| 8932 | Synthesis, chemical characterization, computational studies and biological activity of new DNA methyltransferases (DNMTs) specific inhibitor. Epigenetic regulation as a new and potential approach to cancer therapy. <i>Journal of Inorganic Biochemistry</i> , 2015, 150, 18-27. | 1.5 | 14 |
| 8933 | The Wade-Mingos rules in seven-vertex dimetallaborane chemistry: Hydrogen-rich Cp ₂ M ₂ B ₅ H ₉ systems of the second and third row transition metals. <i>Journal of Organometallic Chemistry</i> , 2015, 792, 74-80. | 0.8 | 3 |
| 8934 | Intermolecular hydrogen bonds in urea-water complexes: DFT, NBO, and AIM analysis. <i>Computational and Theoretical Chemistry</i> , 2015, 1070, 40-47. | 1.1 | 41 |
| 8935 | Representative Amino Acid Side-Chain Interactions in Protein-DNA Complexes: A Comparison of Highly Accurate Correlated <i>Ab Initio</i> Quantum Mechanical Calculations and Efficient Approaches for Applications to Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4086-4092. | 2.3 | 22 |
| 8936 | In Silico Study on the Interaction of Thiazolidinediones and Î ² -Lactoglobulin by Molecular Dynamics and Docking Approach. <i>Journal of Macromolecular Science - Physics</i> , 2015, 54, 1042-1052. | 0.4 | 0 |
| 8937 | Stable structures of LnSi ₆ ⁺ and LnSi ₆ clusters (Ln=Pr, Eu, Gd, Tb, Yb), C _{2v} or C _{5v} ? Explanation of photoelectron spectra. <i>Computational and Theoretical Chemistry</i> , 2015, 1070, 1-8. | 1.1 | 9 |
| 8938 | Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study. <i>Journal of Chemical Thermodynamics</i> , 2015, 91, 186-193. | 1.0 | 31 |
| 8939 | Quantum-Chemical Studies on Excitation Energy Transfer Processes in BODIPY-Based Donor-Acceptor Systems. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4316-4327. | 2.3 | 29 |
| 8940 | Incremental evaluation of coupled cluster dipole polarizabilities. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14284-14296. | 1.3 | 13 |
| 8941 | A simple method for the determination of the Tolman electronic parameter of different phosphorus containing ligands, by means of the average local ionization energy. <i>Inorganica Chimica Acta</i> , 2015, 436, 163-168. | 1.2 | 16 |
| 8942 | Bis(dimethylphosphino)methane-ligated silver chloride, cyanide and hydride cluster cations: Synthesis and gas-phase unimolecular reactivity. <i>International Journal of Mass Spectrometry</i> , 2015, 378, 86-94. | 0.7 | 10 |
| 8943 | Selenocysteine oxidation in glutathione peroxidase catalysis: an MS-supported quantum mechanics study. <i>Free Radical Biology and Medicine</i> , 2015, 87, 1-14. | 1.3 | 100 |
| 8944 | Metallophilic Contacts in 2-C ₆ F ₄ PPh ₂ Bridged Heterobinuclear Complexes: A Crystallographic and Computational Study. <i>Inorganic Chemistry</i> , 2015, 54, 6947-6957. | 1.9 | 13 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 8945 | Conjugate Addition/[3,3] Sigmatropic Shift Processes for Formation of Medium-Ring Cyclic Amines – Do They Circumvent the Woodward–Hoffmann Rules?. <i>Journal of Organic Chemistry</i> , 2015, 80, 11699-11705. | 1.7 | 8 |
| 8946 | The Gilded Edge in Acetylenic Scaffolding II: A Computational Study of the Transmetalation Processes Involved in Palladium-Catalyzed Cross-Couplings of Gold(I) Acetylides. <i>Organometallics</i> , 2015, 34, 3678-3685. | 1.1 | 3 |
| 8947 | Distortion–interaction analysis along the reaction pathway to reveal the reactivity of the Alder-ene reaction of enes. <i>RSC Advances</i> , 2015, 5, 61426-61435. | 1.7 | 27 |
| 8948 | Measuring Propargyl-Linked Drug Populations Inside Bacterial Cells, and Their Interaction with a Dihydrofolate Reductase Target, by Raman Microscopy. <i>Biochemistry</i> , 2015, 54, 2719-2726. | 1.2 | 15 |
| 8949 | Computational Approach to the Study of Epitaxy: Natural Occurrence in Diamond/Forsterite and Aragonite/Zabuyelite. <i>Crystal Growth and Design</i> , 2015, 15, 2979-2987. | 1.4 | 12 |
| 8950 | Flux Synthesis, Structure, Properties, and Theoretical Magnetic Study of Uranium(IV)-Containing $A_2USi_6O_{15}$ ($A = K, Rb$) with an Intriguing Green-to-Purple, Crystal-to-Crystal Structural Transition in the K Analogue. <i>Inorganic Chemistry</i> , 2015, 54, 5504-5511. | 1.9 | 25 |
| 8951 | Improving Rydberg Excitations within Time-Dependent Density Functional Theory with Generalized Gradient Approximations: The Exchange-Enhancement-for-Large-Gradient Scheme. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3123-3130. | 2.3 | 28 |
| 8952 | Reformulation of the D3(Becke–Johnson) Dispersion Correction without Resorting to Higher than C_6 Dispersion Coefficients. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3163-3170. | 2.3 | 83 |
| 8953 | Accurate Infrared (IR) Spectra for Molecules Containing the $C\equiv N$ Moiety by Anharmonic Computations with the Double Hybrid B2PLYP Density Functional. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4364-4369. | 2.3 | 17 |
| 8954 | Thermal Decomposition of NCN: Shock-Tube Study, Quantum Chemical Calculations, and Master-Equation Modeling. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7838-7846. | 1.1 | 14 |
| 8955 | Transition Flux Formula for the Electronic Coupling Matrix Element. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7712-7721. | 1.2 | 8 |
| 8956 | Complexes of a naphthalimide photoacid with organic bases, and their excited-state dynamics in polar aprotic organic solvents. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20715-20724. | 1.3 | 20 |
| 8957 | Natures of optical absorption transitions and excitation energy dependent photostability of diketopyrrolopyrrole (DPP)-based photovoltaic copolymers. <i>Energy and Environmental Science</i> , 2015, 8, 3222-3232. | 15.6 | 90 |
| 8958 | Efficient implementation of the analytic second derivatives of Hartree–Fock and hybrid DFT energies: a detailed analysis of different approximations. <i>Molecular Physics</i> , 2015, 113, 1961-1977. | 0.8 | 38 |
| 8959 | Force field parameters for aminoorganosilanes. <i>Journal of Molecular Structure</i> , 2015, 1079, 363-369. | 1.8 | 4 |
| 8960 | SP20 Phosphorylation Reaction Catalyzed by Protein Kinase A: QM/MM Calculations Based on Recently Determined Crystallographic Structures. <i>ACS Catalysis</i> , 2015, 5, 4897-4912. | 5.5 | 19 |
| 8961 | Electron Localization of Anions Probed by Nitrile Vibrations. <i>Journal of the American Chemical Society</i> , 2015, 137, 10979-10991. | 6.6 | 29 |
| 8962 | How can $[Mo^{IV}(CN)_6]^{2-}$, an apparently octahedral (d^2) complex, be diamagnetic? Insights from quantum chemical calculations and magnetic susceptibility measurements. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14890-14902. | 1.3 | 12 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8963 | Wavelength resolved specific optical rotations and homochiral equilibria. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 21630-21633. | 1.3 | 9 |
| 8964 | Triazine-Substituted and Acyl Hydrazones: Experiment and Computation Reveal a Stability Inversion at Low pH. <i>Molecular Pharmaceutics</i> , 2015, 12, 2924-2927. | 2.3 | 19 |
| 8965 | Theoretical study of the structure of acyclic diaminocarbene ligands in Pd(II) complexes. <i>Russian Journal of General Chemistry</i> , 2015, 85, 894-898. | 0.3 | 4 |
| 8966 | Mechanistic insight into water-modulated cycloisomerization of enynyl esters using an Au(μ) catalyst. <i>Dalton Transactions</i> , 2015, 44, 5354-5363. | 1.6 | 37 |
| 8967 | Mechanistic insight into conjugated N=N bond cleavage by Rh(μ)-catalyzed redox-neutral C-H activation of pyrazolones. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 8251-8260. | 1.5 | 28 |
| 8968 | Electronic structure and thermochemical properties of neutral and anionic rhodium clusters Rh _n , n=2-13. Evolution of structures and stabilities of binary clusters Rh _m M (M=Fe, Co, Ni; m=1-6). <i>Computational and Theoretical Chemistry</i> , 2015, 1068, 30-41. | 1.1 | 15 |
| 8969 | Unexpected electron acceptor behavior of the 1,3,4-thiadiazole oligomer, a DFT study. <i>Computational and Theoretical Chemistry</i> , 2015, 1068, 109-116. | 1.1 | 3 |
| 8970 | Molybdenum Trihydride Complexes: Computational Determinations of Hydrogen Positions and Rearrangement Mechanisms. <i>Inorganic Chemistry</i> , 2015, 54, 6380-6385. | 1.9 | 6 |
| 8971 | Mechanism of Oxygen Activation in a Flavin-Dependent Monooxygenase: A Nearly Barrierless Formation of C4a-Hydroperoxyflavin via Proton-Coupled Electron Transfer. <i>Journal of the American Chemical Society</i> , 2015, 137, 9363-9374. | 6.6 | 70 |
| 8972 | Accuracy of Protein Embedding Potentials: An Analysis in Terms of Electrostatic Potentials. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1832-1842. | 2.3 | 50 |
| 8973 | Redox-Active Sites in <i>Auricularia auricula-judae</i> Dye-Decolorizing Peroxidase and Several Directed Variants: A Multifrequency EPR Study. <i>Journal of Physical Chemistry B</i> , 2015, 119, 13583-13592. | 1.2 | 16 |
| 8974 | Facile Route to the Controlled Synthesis of Tetragonal and Orthorhombic SnO ₂ Films by Mist Chemical Vapor Deposition. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 12074-12079. | 4.0 | 43 |
| 8975 | A kinetic and mechanistic study of dinuclear Pt(II) 2,2':6''-terpyridine compounds bridged with polyethyleneglycol ether flexible linkers. <i>Journal of Coordination Chemistry</i> , 2015, 68, 3013-3031. | 0.8 | 6 |
| 8976 | Four-Component Relativistic Density-Functional Theory Calculations of Nuclear Spin-Rotation Constants: Relativistic Effects in p-Block Hydrides. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3729-3739. | 2.3 | 32 |
| 8977 | Gold(III)-Catalyzed Intramolecular Cyclization of β -Pyrroles to Pyrrolopyridinones and Pyrroloazepinones: A DFT Study. <i>Organometallics</i> , 2015, 34, 3538-3545. | 1.1 | 24 |
| 8978 | Electron Injection from Copper Diimine Sensitizers into TiO ₂ : Structural Effects and Their Implications for Solar Energy Conversion Devices. <i>Journal of the American Chemical Society</i> , 2015, 137, 9670-9684. | 6.6 | 60 |
| 8979 | The relationship between the strength of hydrogen bonding and spin crossover behaviour in a series of iron(μ) Schiff base complexes. <i>Dalton Transactions</i> , 2015, 44, 4474-4484. | 1.6 | 53 |
| 8980 | Development and applications of the LFDDT: the non-empirical account of ligand field and the simulation of the f-d transitions by density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 18547-18557. | 1.3 | 23 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8981 | Highly enantioselective construction of tertiary thioethers and alcohols via phosphine-catalyzed asymmetric \hat{I}^3 -addition reactions of 5H-thiazol-4-ones and 5H-oxazol-4-ones: scope and mechanistic understandings. <i>Chemical Science</i> , 2015, 6, 4912-4922. | 3.7 | 117 |
| 8982 | Active space and basis set effects in $\langle \text{scp} \rangle \text{CASPT} \langle / \text{scp} \rangle 2$ models of the 1,3-butadiene-ethene cycloaddition and the 1,3-butadiene dimerization. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 989-1001. | 1.0 | 4 |
| 8983 | An accurate benchmark description of the interactions between carbon dioxide and polyheterocyclic aromatic compounds containing nitrogen. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 16560-16574. | 1.3 | 30 |
| 8984 | Tetraguanidino-functionalized phenazine and fluorene dyes: synthesis, optical properties and metal coordination. <i>Dalton Transactions</i> , 2015, 44, 3467-3485. | 1.6 | 35 |
| 8985 | A Theoretical Investigation of 1-Butanol Unimolecular Decomposition. <i>Lecture Notes in Computer Science</i> , 2015, , 384-393. | 1.0 | 1 |
| 8986 | Copper(II) complexes with new fluoroquinolones: Synthesis, structure, spectroscopic and theoretical study, DNA damage, cytotoxicity and antiviral activity. <i>Journal of Inorganic Biochemistry</i> , 2015, 150, 160-173. | 1.5 | 30 |
| 8987 | Comparison of Redox Activity between 2-Aminothioether and 2-Aminothiophenol: Redox-Induced Dimerization of 2-Aminothioether via C-C Coupling. <i>Inorganic Chemistry</i> , 2015, 54, 6235-6244. | 1.9 | 5 |
| 8988 | TD-DFT Benchmark on Inorganic Pt(II) and Ir(III) Complexes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3281-3289. | 2.3 | 104 |
| 8989 | Cyclooctatetraenophanes: A Computational Study. <i>Journal of Organic Chemistry</i> , 2015, 80, 6679-6686. | 1.7 | 3 |
| 8990 | Theoretical Rationalization of the Emission Properties of Prototypical Cu(I)-Phenanthroline Complexes. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7026-7037. | 1.1 | 45 |
| 8991 | Derivation of the spin Hamiltonians for Fe in MgO. <i>New Journal of Physics</i> , 2015, 17, 033020. | 1.2 | 17 |
| 8992 | Unique adsorption behaviors of carboxylic acids at rutile TiO ₂ (110). <i>Surface Science</i> , 2015, 641, 82-90. | 0.8 | 17 |
| 8993 | Correlating Photoacidity to Hydrogen-Bond Structure by Using the Local O-H Stretching Probe in Hydrogen-Bonded Complexes of Aromatic Alcohols. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4800-4812. | 1.1 | 26 |
| 8994 | Strong Dependence of Structural and Electronic Properties of Rod-Shaped [RGaNH] ₃ (R = H, CH ₃) Oligomers on Terminal Groups. <i>Journal of Physical Chemistry C</i> , 2015, 119, 16475-16482. | 1.5 | 4 |
| 8995 | Pressure induced effects on the electronic and optical properties of MoS ₂ . <i>Solid State Communications</i> , 2015, 219, 33-38. | 0.9 | 9 |
| 8996 | A computational mechanistic investigation of hydrogen production in water using the [RhIII(dmbpy)2Cl ₂]/[RuII(bpy) ₃] ²⁺ /ascorbic acid photocatalytic system. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10497-10509. | 1.3 | 19 |
| 8997 | Influence of pH and type of counterion on the formation of bismuth(III) complexes with tropolonato and 5-methyltropolonato ligands: Synthesis, structure, spectroscopic characterization and calculation studies. <i>Inorganica Chimica Acta</i> , 2015, 436, 57-68. | 1.2 | 8 |
| 8998 | Synthesis and structure of novel ferrocene-containing \hat{I}^2 -carbolines including polycondensed derivatives with the elements of planar-, central- and conformational chirality. <i>Journal of Organometallic Chemistry</i> , 2015, 794, 125-135. | 0.8 | 5 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 8999 | Synthesis and structures of $[Si(H)P(\frac{1}{4}NR)]_2$, potential building blocks for inorganic phosphorus-sulfur macrocycles. <i>Dalton Transactions</i> , 2015, 44, 14242-14247. | 1.6 | 11 |
| 9000 | Hybrid Functionals with Variationally Fitted Exact Exchange. <i>Advances in Quantum Chemistry</i> , 2015, 71, 41-67. | 0.4 | 11 |
| 9001 | Ruthenium-Catalyzed Deuteration of Alcohols with Deuterium Oxide. <i>Organometallics</i> , 2015, 34, 3686-3698. | 1.1 | 43 |
| 9002 | Cyclopentadienylcobalt azaboranes violating the Wade-Mingos rules: a degree 3 vertex for the nitrogen atom. <i>RSC Advances</i> , 2015, 5, 56885-56890. | 1.7 | 2 |
| 9003 | Influence of mesogenic core polarity and position of chains attachment on columnar phase stability. <i>Liquid Crystals</i> , 0, , 1-13. | 0.9 | 1 |
| 9004 | Electronic and photophysical properties of 2-(2-hydroxyphenyl)benzoxazole and its derivatives enhancing in the excited-state intramolecular proton transfer processes: A TD-DFT study on substitution effect. <i>Journal of Luminescence</i> , 2015, 167, 132-139. | 1.5 | 22 |
| 9005 | Analysis of tautomeric equilibrium in (E)-4,6-dibromo-2-[(4-fluorophenylimino)methyl]-3-methoxyphenol compound. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 731-738. | 2.0 | 5 |
| 9006 | Lewis acidity enhancement of triarylborane by appended phosphine oxide groups. <i>Dalton Transactions</i> , 2015, 44, 4765-4772. | 1.6 | 7 |
| 9007 | Performance of Frozen Density Embedding for Modeling Hole Transfer Reactions. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7541-7557. | 1.2 | 46 |
| 9008 | Insights from the computational studies on the oxidized as-isolated state of [NiFeSe] hydrogenase from <i>D. vulgaris</i> Hildenborough. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20677-20686. | 1.3 | 2 |
| 9009 | Syntheses, structural characterisation and electronic structures of some simple acyclic amino carbene complexes. <i>Dalton Transactions</i> , 2015, 44, 14341-14348. | 1.6 | 19 |
| 9010 | Preparation, electrochemical behavior, and variable-temperature magnetic properties of $Co(3,5-DBSQ)_2$ complexes of imidazole- or pyrazole-substituted ligands. <i>Canadian Journal of Chemistry</i> , 2015, 93, 769-774. | 0.6 | 3 |
| 9011 | Paradox of Self-Interaction Correction. <i>Advances in Atomic, Molecular and Optical Physics</i> , 2015, , 1-14. | 2.3 | 29 |
| 9012 | Synthesis, spectroscopy, electrochemistry, and coordination chemistry of substituted phosphine sulfides and selenides. <i>Polyhedron</i> , 2015, 100, 333-343. | 1.0 | 12 |
| 9013 | The relative stability of mesoionic and N-heterocyclic carbene tautomers: a computational study of substituent effects. <i>Tetrahedron</i> , 2015, 71, 6846-6851. | 1.0 | 14 |
| 9014 | Highly efficient and reversible SO_2 capture by halogenated carboxylate ionic liquids. <i>RSC Advances</i> , 2015, 5, 60975-60982. | 1.7 | 36 |
| 9015 | A BODIPY-based turn-on fluorescent probe for the selective detection of hydrogen sulfide in solution and in cells. <i>Talanta</i> , 2015, 144, 763-768. | 2.9 | 50 |
| 9016 | A Relativistic Quantum-Chemical Analysis of the trans Influence on 1H NMR Hydride Shifts in Square-Planar Platinum(II) Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 7199-7208. | 1.9 | 60 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9017 | Activation Parameters for Additions to Alkenes of Arylchlorocarbenes with Enhanced Electrophilicity. <i>Journal of Organic Chemistry</i> , 2015, 80, 7590-7593. | 1.7 | 10 |
| 9018 | Thermal Cis-to-Trans Isomerization of Azobenzene-Containing Molecules Enhanced by Gold Nanoparticles: An Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 17369-17377. | 1.5 | 52 |
| 9019 | Three different structural lead(II) polymers constructed from newly designed chlorophenyl-imidazole dicarboxylate ligands. <i>Journal of Coordination Chemistry</i> , 2015, 68, 2507-2519. | 0.8 | 6 |
| 9020 | Synthesis of an unexpected [Zn ₂] ²⁺ species utilizing an MFI-type zeolite as a nano-reaction pot and its manipulation with light and heat. <i>Dalton Transactions</i> , 2015, 44, 10038-10047. | 1.6 | 25 |
| 9021 | Coextraction of Water into Nitrobenzene with Organic Ions. <i>Journal of Physical Chemistry B</i> , 2015, 119, 6010-6017. | 1.2 | 9 |
| 9022 | Theoretical design of tetra(arenediyl)bis(allyl) derivatives as model compounds for Cope rearrangement transition states. <i>RSC Advances</i> , 2015, 5, 11494-11497. | 1.7 | 2 |
| 9023 | X-ray Crystallographic, Multifrequency Electron Paramagnetic Resonance, and Density Functional Theory Characterization of the Ni(P ^{Cy}) ₂ N ^{tBu}) ₂ ⁿ Hydrogen Oxidation Catalyst in the Ni(I) Oxidation State. <i>Inorganic Chemistry</i> , 2015, 54, 6226-6234. | 1.9 | 13 |
| 9024 | Comprehensive Benchmark of Association (Free) Energies of Realistic Host-Guest Complexes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3785-3801. | 2.3 | 188 |
| 9025 | An FT-IR and DFT study of the free and solvated 4-(imidazol-1-yl)phenol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 150, 614-622. | 2.0 | 2 |
| 9026 | C ₂ -Symmetric 1,2-di(flourenylidene)cyclobutanes: syntheses, structures, rearrangements and reactivity. <i>Tetrahedron</i> , 2015, 71, 5045-5054. | 1.0 | 0 |
| 9027 | Structural Design Parameters for Highly Birefringent Coordination Polymers. <i>Inorganic Chemistry</i> , 2015, 54, 6462-6471. | 1.9 | 23 |
| 9028 | Calibration of Energy-Specific TDDFT for Modeling K-edge XAS Spectra of Light Elements. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2994-2999. | 2.3 | 78 |
| 9029 | Modeling Cu ₂ +A ²⁺ complexes from computational approaches. <i>AIP Advances</i> , 2015, 5, 092402. | 0.6 | 17 |
| 9030 | Variation in crystalline architectures through supramolecular interactions in copper(II) complexes with tridentate N ₂ O donor Schiff bases. <i>Journal of Coordination Chemistry</i> , 2015, 68, 2520-2538. | 0.8 | 8 |
| 9031 | QM/MM MD Simulations on the Enzymatic Pathway of the Human Flap Endonuclease (hFEN1) Elucidating Common Cleavage Pathways to RNase H Enzymes. <i>ACS Catalysis</i> , 2015, 5, 3864-3875. | 5.5 | 45 |
| 9032 | Liposome-based gene delivery systems containing a steroid derivative: computational and small angle X-ray diffraction study. <i>RSC Advances</i> , 2015, 5, 54070-54078. | 1.7 | 17 |
| 9033 | Nuclear electric quadrupole moment of potassium from the molecular method. <i>Physical Review A</i> , 2015, 91, . | 1.0 | 5 |
| 9034 | Contrasting the optical properties of the different isomers of oligophenylene. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 17854-17863. | 1.3 | 25 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9035 | Tuning the Basicity of Cyano-containing Ionic Liquids to Improve SO ₂ Capture through Cyano-Sulfur Interactions. <i>Chemistry - A European Journal</i> , 2015, 21, 5632-5639. | 1.7 | 55 |
| 9036 | Open-shell doublet character in a hexaazatrinaphthylene trianion complex. <i>Chemical Communications</i> , 2015, 51, 11478-11481. | 2.2 | 23 |
| 9037 | Quantifying N-heterocyclic carbenes as umpolung catalysts in the benzoin reaction: balance between nucleophilicity and electrophilicity. <i>New Journal of Chemistry</i> , 2015, 39, 4508-4518. | 1.4 | 26 |
| 9038 | Spectroscopic and Computational Insights on Catalytic Synergy in Bimetallic Aluminophosphate Catalysts. <i>Journal of the American Chemical Society</i> , 2015, 137, 8534-8540. | 6.6 | 23 |
| 9039 | Design and application of a water-soluble phosphorescent Ru(II) complex as turn-on sensing material for Hg ²⁺ . <i>Journal of Materials Chemistry B</i> , 2015, 3, 6205-6212. | 2.9 | 18 |
| 9040 | Solid-state EPR strategies for the structural characterization of paramagnetic NO adducts of frustrated Lewis pairs (FLPs). <i>Journal of Chemical Physics</i> , 2015, 142, 124201. | 1.2 | 11 |
| 9041 | Generalized vibrational perturbation theory for rovibrational energies of linear, symmetric and asymmetric tops: Theory, approximations, and automated approaches to deal with medium-to-large molecular systems. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 948-982. | 1.0 | 95 |
| 9042 | Mechanism of palladium(II)-catalyzed reaction between styrene and carbazole. <i>Computational and Theoretical Chemistry</i> , 2015, 1068, 47-51. | 1.1 | 3 |
| 9043 | Spectroscopic characterization and density functional studies of (Z)-1-[(2-methoxy-5-(trifluoromethyl)phenylamino)methylene]naphthalene-2(1H)-one. <i>Journal of Molecular Structure</i> , 2015, 1097, 171-180. | 1.8 | 28 |
| 9044 | Molecular mechanics and quantum chemistry evaluation of the effect of the side chain structure of brassinosteroids on their biological activity. <i>Journal of Structural Chemistry</i> , 2015, 56, 330-337. | 0.3 | 2 |
| 9045 | Photoisomerization action spectroscopy: flicking the protonated merocyanine-spiropyran switch in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 25676-25688. | 1.3 | 46 |
| 9046 | Anharmonic simulations of the vibrational spectrum of sulfated compounds: application to the glycosaminoglycan fragment glucosamine 6-sulfate. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 25705-25713. | 1.3 | 33 |
| 9047 | Electron Ionization Mass Spectrum of Tellurium Hexafluoride. <i>Inorganic Chemistry</i> , 2015, 54, 4821-4826. | 1.9 | 6 |
| 9048 | Absolute Reactivity of (N-Methyl-3-pyridinium)chlorocarbene. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3556-3562. | 1.1 | 7 |
| 9049 | H and D Attachment to Naphthalene: Spectra and Thermochemistry of Cold Gas-Phase 1-C ₁₀ H ₉ and 1-C ₁₀ H ₈ D Radicals and Cations. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3225-3232. | 1.1 | 10 |
| 9050 | Validation of Methods for Computational Catalyst Design: Geometries, Structures, and Energies of Neutral and Charged Silver Clusters. <i>Journal of Physical Chemistry C</i> , 2015, 119, 9617-9626. | 1.5 | 31 |
| 9051 | Hydrogen Trapping Ability of the Pyridine-Lithium ⁺ (1:1) Complex. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3056-3063. | 1.1 | 18 |
| 9052 | Implication of a η^5 -Methane Complex en Route to Elimination of Methane from a Ruthenium Complex: An Experimental and Theoretical Investigation. <i>Organometallics</i> , 2015, 34, 1245-1254. | 1.1 | 10 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9053 | Al Atom Activation of C–S Bonds: Characterization of the Aluminathietane Formed in the Reaction of Al Atoms with 1,2-Butylene Sulfide. <i>Organometallics</i> , 2015, 34, 1264-1271. | 1.1 | 2 |
| 9054 | Fe(II)-Polypyridines as Chromophores in Dye-Sensitized Solar Cells: A Computational Perspective. <i>Accounts of Chemical Research</i> , 2015, 48, 1441-1449. | 7.6 | 76 |
| 9055 | The Mechanism of Pyrolysis of Benzyl Azide: Spectroscopic Evidence for Benzenemethanimine Formation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4118-4126. | 1.1 | 9 |
| 9056 | Urea enhances the photodynamic efficiency of methylene blue. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2015, 150, 31-37. | 1.7 | 45 |
| 9057 | Bonding nature of the actinide tetrafluorides AnF_4 ($An = Th, Cm$). <i>Molecular Physics</i> , 2015, 113, 3450-3458. | 0.8 | 6 |
| 9058 | Theoretical investigations into the electronic structures and electron transport properties of fluorine and carbonyl end-functionalized quarterthiophenes. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 59, 50-58. | 1.3 | 2 |
| 9059 | Low cost, ultra-thin films of reduced graphene oxide–Ag nanoparticle hybrids as SERS based excellent dye sensors. <i>Chemical Physics Letters</i> , 2015, 629, 81-86. | 1.2 | 34 |
| 9060 | Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against structure calculations and experiments. <i>Physical Review B</i> , 2015, 91, . | 1.1 | 140 |
| 9061 | A Practicable Real Space Measure and Visualization of Static Electron–Correlation Effects. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 12308-12313. | 7.2 | 194 |
| 9062 | Kondo Effect in a Neutral and Stable All Organic Radical Single Molecule Break Junction. <i>Nano Letters</i> , 2015, 15, 3109-3114. | 4.5 | 117 |
| 9063 | A mechanistic study of $Pd(OAc)_2$ -catalyzed intramolecular C–H functionalization reaction involving CO/isonitrile insertion. <i>Dalton Transactions</i> , 2015, 44, 9839-9846. | 1.6 | 7 |
| 9064 | Carbon Dioxide Promoted H_2 Reduction Using a Bis(imino)pyridine Manganese Electrocatalyst. <i>Inorganic Chemistry</i> , 2015, 54, 4475-4482. | 1.9 | 45 |
| 9065 | Inelastic and elastic neutron scattering studies of the vibrational and reorientational dynamics, crystal structure and solid phase transition in $[Mn(OS(CH_3)_2)_6](ClO_4)_2$ supported by theoretical (DFT) calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 145, 368-375. | 2.0 | 6 |
| 9066 | Novel stable phosphastannapropene derivatives. Synthesis and Characterization. <i>Journal of Organometallic Chemistry</i> , 2015, 787, 14-18. | 0.8 | 1 |
| 9067 | The 6,6-Dicyanopentafulvene Core: A Template for the Design of Electron-Acceptor Compounds. <i>Chemistry - A European Journal</i> , 2015, 21, 8168-8176. | 1.7 | 13 |
| 9068 | Vibrational study, molecular properties and first-order molecular hyperpolarizability of Methyl 2-amino 5-bromobenzoate using DFT method. <i>Optical Materials</i> , 2015, 46, 154-167. | 1.7 | 13 |
| 9069 | Exploring the influence of electron donating/withdrawing groups on hexamolybdate-based derivatives for efficient p-type dye-sensitized solar cells (DSSCs). <i>RSC Advances</i> , 2015, 5, 39821-39827. | 1.7 | 30 |
| 9070 | Mechanism of Oxidation of Ethane to Ethanol at Iron(IV)–Oxo Sites in Magnesium-Diluted Fe_2O_3 (dobdc). <i>Journal of the American Chemical Society</i> , 2015, 137, 5770-5781. | 6.6 | 156 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9072 | Infrared spectra of small anionic water clusters from density functional theory and wavefunction theory calculations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12698-12707. | 1.3 | 4 |
| 9073 | Fluorescent benzene-centered mono-, bis- and tris-triazapentadieneâ€“boron complexes. <i>Dalton Transactions</i> , 2015, 44, 9659-9671. | 1.6 | 22 |
| 9074 | Photophysical studies of the interactions of poly(amidoamine) generation zero (PAMAM G0) with copper and zinc ions. <i>Journal of Luminescence</i> , 2015, 164, 23-30. | 1.5 | 6 |
| 9075 | What Makes a Strong Organic Electron Donor (or Acceptor)?. <i>Chemistry - A European Journal</i> , 2015, 21, 8578-8590. | 1.7 | 75 |
| 9076 | Computational Insight into Nickelâ€“Catalyzed Carbonâ€“Carbon versus Carbonâ€“Boron Coupling Reactions of Primary, Secondary, and Tertiary Alkyl Bromides. <i>Chemistry - A European Journal</i> , 2015, 21, 7480-7488. | 1.7 | 43 |
| 9077 | Computational Benchmarking for Ultrafast Electron Dynamics: Wave Function Methods vs Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2221-2233. | 2.3 | 11 |
| 9078 | Acidâ€“base effects, light emission, DNA-binding and photocleavage studies of oligo-homonuclear ruthenium(II) complexes and their computational study. <i>Inorganica Chimica Acta</i> , 2015, 432, 158-168. | 1.2 | 6 |
| 9079 | Experimental and theoretical study of carbohydrateâ€“ionic liquid interactions. <i>Carbohydrate Polymers</i> , 2015, 127, 316-324. | 5.1 | 24 |
| 9080 | Stable porous crystalline silicon with nanotubular structure: A predicted allotrope with direct band gap. <i>Physica B: Condensed Matter</i> , 2015, 466-467, 59-63. | 1.3 | 11 |
| 9081 | Dinuclear and polymeric ($\frac{1}{4}$ -formate)nickel(II) complexes: Synthesis, structure, spectral and magnetic properties. <i>Polyhedron</i> , 2015, 95, 45-53. | 1.0 | 8 |
| 9082 | Vibrational analysis of $\hat{\pm}$ -cyanohydroxycinnamic acid. <i>Journal of Molecular Structure</i> , 2015, 1094, 203-209. | 1.8 | 8 |
| 9083 | A novel Zn(II) complex of N-nicotinyl phosphoramidate: Combined experimental and computational studies. <i>Journal of Molecular Structure</i> , 2015, 1092, 130-136. | 1.8 | 11 |
| 9084 | Reaction pathway and free energy barrier for urea elimination in aqueous solution. <i>Chemical Physics Letters</i> , 2015, 625, 143-146. | 1.2 | 7 |
| 9085 | Mechanical properties and electronic structures of the Hfâ€“Si system: First-principles calculations. <i>Solid State Communications</i> , 2015, 205, 39-45. | 0.9 | 14 |
| 9086 | Elucidating Lewis acidity of metal sites in MFU-4l metal-organic frameworks: N ₂ O and CO ₂ adsorption in MFU-4l, CuI-MFU-4l and Li-MFU-4l. <i>Microporous and Mesoporous Materials</i> , 2015, 216, 146-150. | 2.2 | 21 |
| 9087 | Solid-State NMR Study of Paramagnetic Bis(alaninato- \hat{p} ² _N , _O)copper(II) and Bis(1-amino(cyclo)alkane-1-carboxylato- \hat{p} ² _N , _O)copper(II) Complexes: Reflection of Stereoisomerism and Molecular Mobility in ¹³ C and ² H Fast Magic Angle Spinning Spectra. <i>Inorganic Chemistry</i> , 2015, 54, 4663-4677. | 1.9 | 14 |
| 9088 | Tetracarba- nido- hexa-, -octa, and -decaborane derivatives. NMR study and DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2015, 798, 268-273. | 0.8 | 8 |
| 9089 | Oxidation of Graphene-Edge Six- and Five-Member Rings by Molecular Oxygen. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7528-7547. | 1.1 | 46 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9090 | The Unexpected Mechanism Underlying the High-Valent Mono-oxo-Rhenium(V) Hydride Catalyzed Hydrosilylation of C=C/N Functionalities: Insights from a DFT Study. <i>ChemPhysChem</i> , 2015, 16, 1052-1060. | 1.0 | 5 |
| 9091 | Theoretical exploration to the cation effect on the second-order nonlinear optical properties of Strandberg-type polyoxometalates. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550007. | 1.8 | 2 |
| 9092 | Zinc(II)-methimazole complexes: synthesis and reactivity. <i>Dalton Transactions</i> , 2015, 44, 9805-9814. | 1.6 | 7 |
| 9093 | Origins of Initiation Rate Differences in Ruthenium Olefin Metathesis Catalysts Containing Chelating Benzylidenes. <i>Journal of the American Chemical Society</i> , 2015, 137, 5782-5792. | 6.6 | 89 |
| 9094 | Effect of oxygen content and charge on the structure, stability and optoelectronic properties of yttrium oxide clusters. <i>Journal of Physics and Chemistry of Solids</i> , 2015, 82, 91-100. | 1.9 | 7 |
| 9095 | Near infrared-emitting tris-bidentate Os(II) phosphors: control of excited state characteristics and fabrication of OLEDs. <i>Journal of Materials Chemistry C</i> , 2015, 3, 4910-4920. | 2.7 | 52 |
| 9096 | Theoretical investigation on SnCl ₄ -catalyzed tandem dimerization/oxy-2-azonia-Cope rearrangements between β,β -unsaturated ketones and imines. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1. | 0.5 | 1 |
| 9097 | Why 1,2-quinone derivatives are more stable than their 2,3-analogues?. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1. | 0.5 | 16 |
| 9098 | Computational studies of water and carbon dioxide interactions with cellobiose. <i>Journal of Molecular Modeling</i> , 2015, 21, 16. | 0.8 | 8 |
| 9099 | Synthesis, Characterization and Crystal Structures of Some Metal Carbonyl Linking Clusters of Osmium, Ruthenium and Cobalt Derived from Diethynylarenes. <i>Journal of Cluster Science</i> , 2015, 26, 291-307. | 1.7 | 3 |
| 9100 | DFT Studies of the Photophysical Properties of Fluorescent and Semiconductor Polycyclic Benzimidazole Derivatives. <i>Journal of Fluorescence</i> , 2015, 25, 685-694. | 1.3 | 13 |
| 9101 | Radical-mediated graft modification of polyethylene models with vinyltrimethoxysilane: a theoretical analysis. <i>Structural Chemistry</i> , 2015, 26, 97-107. | 1.0 | 1 |
| 9102 | A DFT study on the mechanism of palladium-catalyzed divergent reactions of 1,6-enyne carbonates. <i>Journal of Chemical Sciences</i> , 2015, 127, 547-556. | 0.7 | 3 |
| 9103 | Structural elucidation and molecular docking of ferulic acid from <i>Parthenium hysterophorus</i> possessing COX-2 inhibition activity. <i>3 Biotech</i> , 2015, 5, 541-551. | 1.1 | 34 |
| 9104 | Formation of a ¹⁺ Ions Directly from Oxazolone b ²⁺ Ions: an Energy-Resolved and Computational Study. <i>Journal of the American Society for Mass Spectrometry</i> , 2015, 26, 774-781. | 1.2 | 17 |
| 9105 | Protonated Hexaazamacrocycles as Selective K ⁺ Receptors. <i>Journal of the American Society for Mass Spectrometry</i> , 2015, 26, 1186-1190. | 1.2 | 4 |
| 9106 | Postsynthetic Metal and Ligand Exchange in MFU-4L: A Screening Approach toward Functional Metal-Organic Frameworks Comprising Single-Site Active Centers. <i>Chemistry - A European Journal</i> , 2015, 21, 8188-8199. | 1.7 | 70 |
| 9107 | Synthesis, Structure, and Reactivity of Anionic sp ² -sp ³ Diboron Compounds: Readily Accessible Boryl Nucleophiles. <i>Chemistry - A European Journal</i> , 2015, 21, 7082-7098. | 1.7 | 175 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9108 | Quantitatively Mapping Cellular Viscosity with Detailed Organelle Information via a Designed PET Fluorescent Probe. <i>Scientific Reports</i> , 2014, 4, 5418. | 1.6 | 109 |
| 9109 | Analysis and Calculation of Electronic Properties and Light Absorption of Defective Sulfur-Doped Silicon and Theoretical Photoelectric Conversion Efficiency. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3753-3761. | 1.1 | 11 |
| 9110 | Assessment of Hybrid Density Functionals for the Adsorption of Carbon Monoxide on Platinum Model Clusters. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4051-4056. | 1.1 | 16 |
| 9111 | AlCl ₃ -Catalyzed Ring Expansion Cascades of Bicyclic Cyclobutenamides Involving Highly Strained <i>cis</i> , <i>trans</i> -Cycloheptadienone Intermediates. <i>Journal of the American Chemical Society</i> , 2015, 137, 5596-5601. | 6.6 | 31 |
| 9112 | Quantum chemical study of intramolecular rearrangements of the cyclooctatetraene complexes C ₈ H ₈ X (X = Mg, Si, S). <i>Russian Journal of Organic Chemistry</i> , 2015, 51, 295-300. | 0.3 | 0 |
| 9113 | Study of the Preparation of Amorphous Itraconazole Formulations. <i>Crystal Growth and Design</i> , 2015, 15, 2686-2694. | 1.4 | 9 |
| 9114 | Benzimidazole-Containing Porous Organic Polymers as Highly Active Heterogeneous Solid-Base Catalysts. <i>ChemCatChem</i> , 2015, 7, 1559-1565. | 1.8 | 29 |
| 9115 | Delocalization of Charge and Electron Density in the Humulyl Cation—Implications for Terpene Biosynthesis. <i>Journal of Organic Chemistry</i> , 2015, 80, 4046-4053. | 1.7 | 14 |
| 9116 | Effect of the nature of non-bridging donor atoms on the structure and magnetic properties of binuclear copper(II) complexes with heterocyclic azomethyne ligands. <i>Journal of Structural Chemistry</i> , 2015, 56, 113-120. | 0.3 | 16 |
| 9117 | Characterizing the Intermediates Compound I and II in the Cytochrome P450 Catalytic Cycle with Nonlinear X-ray Spectroscopy: A Simulation Study. <i>ChemPhysChem</i> , 2015, 16, 2006-2014. | 1.0 | 5 |
| 9118 | N-2-Aryl-1,2,3-Triazoles: A Novel Class of Blue Emitting Fluorophores-Synthesis, Photophysical Properties Study and DFT Computations. <i>Journal of Fluorescence</i> , 2015, 25, 985-996. | 1.3 | 16 |
| 9119 | Dual Fluorescence through Kasha's Rule Breaking: An Unconventional Photomechanism for Intracellular Probe Design. <i>Journal of Physical Chemistry B</i> , 2015, 119, 6144-6154. | 1.2 | 76 |
| 9120 | Synthesis Characterization and DFT Calculations of 2,5-Substituted Thiophene Derivatives. <i>Journal of Chemical Crystallography</i> , 2015, 45, 238-243. | 0.5 | 8 |
| 9121 | Structure and Chemistry of SeF _x (CN) _{4-x} Compounds. <i>Inorganic Chemistry</i> , 2015, 54, 5220-5231. | 1.9 | 12 |
| 9122 | Coordination properties of a metal chelator clioquinol to Zn ²⁺ studied by static DFT and ab initio molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13582-13589. | 1.3 | 13 |
| 9123 | Stable Iridium(IV) Complexes of an Oxidation-Resistant Pyridine-Alkoxide Ligand: Highly Divergent Redox Properties Depending on the Isomeric Form Adopted. <i>Journal of the American Chemical Society</i> , 2015, 137, 7243-7250. | 6.6 | 51 |
| 9124 | Comparative study of small boron, silicon and germanium clusters: B _m Si _n and B _m Ge _n (m + n = 2-4). <i>Journal of Molecular Modeling</i> , 2015, 21, 141. | 0.8 | 8 |
| 9125 | Protonated heterocyclic derivatives of cyclopropane and cyclopropanone: classical species, alternate sites, and ring fragmentation. <i>Canadian Journal of Chemistry</i> , 2015, 93, 708-714. | 0.6 | 5 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9126 | Benzimidazolium-based chemosensors: selective recognition of $H_2PO_4^-$, $HP_2O_7^{3-}$, F^- and ATP through fluorescence and gelation studies. <i>RSC Advances</i> , 2015, 5, 46608-46616. | 1.7 | 19 |
| 9127 | Computational and Experimental Investigations of the Formal Dyotropic Rearrangements of Himbert Arene/Allene Cycloadducts. <i>Journal of the American Chemical Society</i> , 2015, 137, 6956-6964. | 6.6 | 16 |
| 9128 | Octacoordinated Dioxo-Molybdenum Complex via Formal Oxidative Addition of Molecular Oxygen. Studies of Chemical Reactions Between $M(CO)_6$ ($M = Cr, Mo$) and 2,4-Di- <i>tert</i> -butyl-6-(pyridin-2-ylazo)-phenol. <i>Inorganic Chemistry</i> , 2015, 54, 5257-5265. | 1.9 | 19 |
| 9129 | Five-Photon Absorption and Selective Enhancement of Multiphoton Absorption Processes. <i>ACS Photonics</i> , 2015, 2, 572-577. | 3.2 | 16 |
| 9130 | Hybrid functional band gap calculation of SnO_6 containing perovskites and their derived structures. <i>Journal of Solid State Chemistry</i> , 2015, 228, 214-220. | 1.4 | 8 |
| 9131 | Visible and Ultraviolet Spectroscopy of Gas Phase Rhodamine 575 Cations. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5634-5641. | 1.1 | 14 |
| 9132 | Spectroscopic and theoretical studies of bis(dimethylphenyl betaine) hydrochloride monohydrate. <i>Vibrational Spectroscopy</i> , 2015, 79, 16-23. | 1.2 | 8 |
| 9133 | Linker dependence of interfacial electron transfer rates in Fe(II)-polypyridine sensitized solar cells. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 134205. | 0.7 | 19 |
| 9134 | Electronically excited states of PANH anions. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14761-14772. | 1.3 | 23 |
| 9135 | Palladium(II) Complex of a Redox-Active Amidophenolate-Based O, N, S, N Ligand: Its Monocation and Dication and Reactivity with PPh_3 . <i>Inorganic Chemistry</i> , 2015, 54, 5182-5194. | 1.9 | 31 |
| 9136 | Synthesis, Electrochemistry, and Single-Molecule Conductance of Bimetallic 2,3,5,6-Tetra(pyridine-2-yl)pyrazine-Based Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 5487-5494. | 1.9 | 37 |
| 9137 | Do Practical Standard Coupled Cluster Calculations Agree Better than Kohn-Sham Calculations with Currently Available Functionals When Compared to the Best Available Experimental Data for Dissociation Energies of Bonds to 3d Transition Metals?. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2036-2052. | 2.3 | 109 |
| 9138 | ReaxFF Reactive Molecular Dynamics Simulation of the Hydration of Cu-SSZ-13 Zeolite and the Formation of Cu Dimers. <i>Journal of Physical Chemistry C</i> , 2015, 119, 6678-6686. | 1.5 | 78 |
| 9139 | Intra- and Intermolecular Dispersion Interactions in $[n]$ Cycloparaphenylenes: Do They Influence Their Structural and Electronic Properties?. <i>ChemPhysChem</i> , 2015, 16, 1520-1528. | 1.0 | 15 |
| 9140 | Infrared spectra of formic acid clusters in noble gas matrices. <i>Journal of Molecular Structure</i> , 2015, 1091, 203-209. | 1.8 | 18 |
| 9141 | Thiolate-Bridged Dinuclear Ruthenium and Iron Complexes as Robust and Efficient Catalysts toward Oxidation of Molecular Dihydrogen in Protic Solvents. <i>Journal of the American Chemical Society</i> , 2015, 137, 4173-4182. | 6.6 | 19 |
| 9142 | Quantitative prediction of charge mobilities of π -stacked systems by first-principles simulation. <i>Nature Protocols</i> , 2015, 10, 632-642. | 5.5 | 187 |
| 9143 | Regioselectivity in Ligand Substitution Reactions on Diiron Complexes Governed by Nucleophilic and Electrophilic Ligand Properties. <i>Inorganic Chemistry</i> , 2015, 54, 3523-3535. | 1.9 | 12 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9144 | Structure and Vibrational Spectra of Uranyl Dinitrate Complexes with Water and DMSO. <i>Journal of Applied Spectroscopy</i> , 2015, 82, 25-32. | 0.3 | 2 |
| 9145 | Dimetallaborane analogues of pentaborane. <i>Dalton Transactions</i> , 2015, 44, 7355-7363. | 1.6 | 2 |
| 9146 | On the Basicity of 8-Phenylsulfanyl Quipazine Derivatives: New Potential Serotonergic Agents. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6989-6999. | 1.1 | 1 |
| 9147 | Biodegradable betaine-based aprotic task-specific ionic liquids and their application in efficient SO ₂ absorption. <i>Green Chemistry</i> , 2015, 17, 3798-3805. | 4.6 | 40 |
| 9148 | [P ₃ Se ₄] ⁺ : A Binary Phosphorus–Selenium Cation. <i>Chemistry - A European Journal</i> , 2015, 21, 9697-9712. | 1.7 | 19 |
| 9149 | What factors cause the complete substrate-controlled selectivity in Rh ₂ (Piv) ₄ -catalyzed cycloadditions of 1,2,3-triazoles with isocyanates or isothiocyanates. <i>Journal of Organometallic Chemistry</i> , 2015, 788, 58-67. | 0.8 | 2 |
| 9150 | Novel water soluble neutral vanadium(IV)–antibiotic complex: Antioxidant, immunomodulatory and molecular docking studies. <i>European Journal of Medicinal Chemistry</i> , 2015, 97, 214-224. | 2.6 | 21 |
| 9151 | Benzothiadiazole-based organic dyes with pyridine anchors for dye-sensitized solar cells: effect of donor on optical properties. <i>Tetrahedron</i> , 2015, 71, 4203-4212. | 1.0 | 38 |
| 9152 | Syntheses, structural diversity and properties of three coordination polymers built by chlorophenyl imidazole dicarboxylate. <i>Supramolecular Chemistry</i> , 2015, 27, 141-150. | 1.5 | 4 |
| 9153 | Imido-pyridine Ti(IV) compounds: synthesis of unusual imido–amido heterobimetallic derivatives. <i>Dalton Transactions</i> , 2015, 44, 11119-11128. | 1.6 | 4 |
| 9154 | Regarding the use and misuse of retinal protonated Schiff base photochemistry as a test case for time-dependent density-functional theory. <i>Journal of Chemical Physics</i> , 2015, 142, 144104. | 1.2 | 15 |
| 9155 | The study of the electronic structure of some N-heterocyclic carbenes (NHCs) by variable energy photoelectron spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10656-10667. | 1.3 | 13 |
| 9156 | Structural, Magnetic, and Redox Diversity of First-Row Transition Metal Complexes of a Pyridine-Based Macrocyclic: Well-Marked Trends Supported by Theoretical DFT Calculations. <i>Inorganic Chemistry</i> , 2015, 54, 3352-3369. | 1.9 | 39 |
| 9157 | Phonon Modes of Organic Electro-Optic Molecular Crystals for Terahertz Photonics. <i>Journal of Physical Chemistry C</i> , 2015, 119, 10031-10039. | 1.5 | 20 |
| 9158 | Spin Propensities of Octahedral Complexes From Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4041-4050. | 1.1 | 80 |
| 9159 | Density Functional Theory Study of the Mechanisms of Iron-Catalyzed Intramolecular C–H Amination [1,2]-Shift Tandem Reactions of Aryl Azides. <i>Organometallics</i> , 2015, 34, 1129-1136. | 1.1 | 14 |
| 9160 | A Quantum Monte Carlo Study of the Reactions of CH with Acrolein. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4214-4223. | 1.1 | 28 |
| 9161 | Beyond Local Group Modes in Vibrational Sum Frequency Generation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3407-3414. | 1.1 | 18 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9162 | N-Heterocyclic Carbene-Catalyzed Ring Opening Polymerization of ϵ -Caprolactone with and without Alcohol Initiators: Insights from Theory and Experiment. <i>Journal of Physical Chemistry B</i> , 2015, 119, 5728-5737. | 1.2 | 38 |
| 9163 | Investigation of the ion signal decay in the reaction region of a pulsed ion mobility spectrometer. <i>International Journal for Ion Mobility Spectrometry</i> , 2015, 18, 41-49. | 1.4 | 4 |
| 9164 | Understanding the Origin of the VCD Signals on the Basis of a Nonredundant Coordinate Definition. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2633-2641. | 2.3 | 2 |
| 9165 | Synthesis, spectroscopic (UV-vis and GIAO NMR), crystallographic and theoretical studies of triazine heterocyclic derivatives. <i>Journal of Molecular Structure</i> , 2015, 1096, 29-37. | 1.8 | 7 |
| 9166 | Using bonding to guide transition state optimization. <i>Journal of Computational Chemistry</i> , 2015, 36, 1157-1166. | 1.5 | 17 |
| 9167 | Dihydrogen Bond Intermediated Alcoholysis of Dimethylamine-Borane in Nonaqueous Media. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3853-3868. | 1.1 | 22 |
| 9168 | Experimental and Theoretical Investigation of SO_2 Adsorption over the 1,3-Phenylenediamine/ SiO_2 System. <i>Journal of Physical Chemistry C</i> , 2015, 119, 6713-6727. | 1.5 | 23 |
| 9169 | Accurate calculation of ^{31}P NMR chemical shifts in polyoxometalates. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8723-8731. | 1.3 | 25 |
| 9170 | Heterolytic Activation of C-H Bonds on Cr^{III} -O Surface Sites Is a Key Step in Catalytic Polymerization of Ethylene and Dehydrogenation of Propane. <i>Inorganic Chemistry</i> , 2015, 54, 5065-5078. | 1.9 | 103 |
| 9171 | General Reaction Mode of Hypervalent Iodine Trifluoromethylation Reagent: A Density Functional Theory Study. <i>ACS Catalysis</i> , 2015, 5, 2458-2468. | 5.5 | 81 |
| 9172 | Molecular properties in the Tamm-Dancoff approximation: indirect nuclear spin-spin coupling constants. <i>Molecular Physics</i> , 2015, 113, 1937-1951. | 0.8 | 9 |
| 9173 | Beyond Energies: Geometries of Nonbonded Molecular Complexes as Metrics for Assessing Electronic Structure Approaches. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1481-1492. | 2.3 | 90 |
| 9174 | Deriving Chemically Essential Interactions Based on Active Site Alignments and Quantum Chemical Calculations: A Case Study on Glycoside Hydrolases. <i>ACS Catalysis</i> , 2015, 5, 2559-2572. | 5.5 | 8 |
| 9175 | Tuning the electronic and magnetic properties of graphene-like AlN nanosheets by surface functionalization and thickness. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10919-10924. | 1.3 | 29 |
| 9176 | The trans-cis and the azide-tetrazole ring-chain isomerization of 2-azido-1,3-azoles: Quantum chemical study. <i>Journal of Molecular Structure</i> , 2015, 1093, 65-76. | 1.8 | 19 |
| 9177 | Conformational landscape and low lying excited states of imatinib. <i>Journal of Molecular Modeling</i> , 2015, 21, 84. | 0.8 | 5 |
| 9178 | Feasibility of Intramolecular Proton Transfers in Terpene Biosynthesis - Guiding Principles. <i>Journal of the American Chemical Society</i> , 2015, 137, 4134-4140. | 6.6 | 31 |
| 9179 | A study of N-trinitroethyl-substituted aminofurazans: high detonation performance energetic compounds with good oxygen balance. <i>Journal of Materials Chemistry A</i> , 2015, 3, 8156-8164. | 5.2 | 56 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9180 | A detailed analysis of the mechanism of a carbocationic triple shift rearrangement. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9771-9779. | 1.3 | 24 |
| 9181 | Conformation change of opiorphin derivatives. A theoretical study of the radical initiated epimerization of opiorphin. <i>Chemical Physics Letters</i> , 2015, 626, 29-38. | 1.2 | 0 |
| 9182 | A crossed molecular beam and ab initio study on the formation of 5- and 6-methyl-1,4-dihydronaphthalene (C ₁₁ H ₁₂) via the reaction of meta-tolyl (C ₇ H ₇) with 1,3-butadiene (C ₄ H ₆). <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7699-7706. | 1.3 | 7 |
| 9183 | Linear Photophysics, Stimulated Emission, and Ultrafast Spectroscopy of New Two-Photon Absorbing Diketopyrrolopyrrole Derivatives. <i>Journal of Physical Chemistry C</i> , 2015, 119, 8864-8875. | 1.5 | 16 |
| 9184 | Theoretical studies on the activation mechanism involving bifunctional tertiary amine-thioureas and isatylidene malononitriles. <i>RSC Advances</i> , 2015, 5, 34314-34318. | 1.7 | 6 |
| 9185 | Understanding the Effects of Bidentate Directing Groups: A Unified Rationale for sp ² and sp ³ C-H Bond Activations. <i>Journal of Organic Chemistry</i> , 2015, 80, 4672-4682. | 1.7 | 58 |
| 9186 | Redox processes of 2,6-dichlorophenolindophenolate in different solvents. A combined electrochemical, spectroelectrochemical, photochemical, and theoretical study. <i>Journal of Solid State Electrochemistry</i> , 2015, 19, 2633-2642. | 1.2 | 8 |
| 9187 | The DFT local reactivity descriptors of Î±-tocopherol. <i>Journal of Molecular Modeling</i> , 2015, 21, 99. | 0.8 | 16 |
| 9188 | Fluorescence Properties of Diphenylthiazolo[4,5-b <i>z</i>]pyrazines Tuned by Donor-Acceptor Substituent Effects. <i>Photochemistry and Photobiology</i> , 2015, 91, 807-813. | 1.3 | 8 |
| 9189 | Inhibition of a multiproduct terpene synthase from <i>Medicago truncatula</i> by 3-bromoprenyl diphosphates. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 4776-4784. | 1.5 | 4 |
| 9190 | Big Data Meets Quantum Chemistry Approximations: The Î”-Machine Learning Approach. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2087-2096. | 2.3 | 579 |
| 9191 | Effect of water treatment on Sn-BEA zeolite: Origin of 960 cm ⁻¹ FTIR peak. <i>Microporous and Mesoporous Materials</i> , 2015, 210, 69-76. | 2.2 | 66 |
| 9192 | Renewable Î²-myrcene polymerization initiated by lutetium alkyl complexes ligated by imidophosphonamido ligand. <i>Chinese Journal of Polymer Science (English Edition)</i> , 2015, 33, 792-796. | 2.0 | 24 |
| 9193 | ¹ H Chemical Shifts in Paramagnetic Co(II) Pyrazolylborate Complexes: A First-Principles Study. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1683-1691. | 2.3 | 52 |
| 9194 | Sequential palladium catalyzed coupling-cyclocondensation-coupling (C ³) four-component synthesis of intensively blue luminescent biarylsubstituted pyrazoles. <i>RSC Advances</i> , 2015, 5, 33838-33854. | 1.7 | 32 |
| 9195 | Nonseparable exchange-correlation functional for molecules, including homogeneous catalysis involving transition metals. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12146-12160. | 1.3 | 111 |
| 9196 | Valence Virtual Orbitals: An Unambiguous ab Initio Quantification of the LUMO Concept. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10408-10427. | 1.1 | 52 |
| 9197 | DFT predictions of the oxidation potential of organic dyes for opto-electronic devices. <i>Computational and Theoretical Chemistry</i> , 2015, 1070, 68-75. | 1.1 | 11 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9198 | Quantum chemical protocols for modeling reactions and spectra in astrophysical ice analogs: the challenging case of the $C^{+} + H_2O$ reaction in icy grain mantles. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28705-28718. | 1.3 | 8 |
| 9199 | Synthesis, structure, and reactivity of iridium perfluorocarbene complexes: regio- and stereo-specific addition of HCl across a metal carbon double bond. <i>Dalton Transactions</i> , 2015, 44, 19528-19542. | 1.6 | 6 |
| 9200 | Cation-Controlled Enantioselective and Diastereoselective Synthesis of Indolines: An Autoinductive Phase-Transfer Initiated 5-endo-trig Process. <i>Journal of the American Chemical Society</i> , 2015, 137, 13414-13424. | 6.6 | 43 |
| 9201 | Ionization and Fragmentation of Formamide Induced by Synchrotron Radiation in the Valence Region via Photoelectron Photoion Coincidence Measurements and Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10300-10308. | 1.1 | 8 |
| 9202 | Birnessite: A Layered Manganese Oxide To Capture Sunlight for Water-Splitting Catalysis. <i>Journal of Physical Chemistry C</i> , 2015, 119, 22838-22846. | 1.5 | 75 |
| 9203 | Structural and spectral properties of tartrato complexes of vanadium(V) from quantum chemical calculations. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1. | 0.5 | 0 |
| 9204 | $P(\dot{O})H$ to $P=OH$ Tautomerism: A Theoretical and Experimental Study. <i>Journal of Organic Chemistry</i> , 2015, 80, 10025-10032. | 1.7 | 114 |
| 9205 | How to make a porphyrin flip: dynamics of asymmetric porphyrin oligomers. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 27094-27102. | 1.3 | 1 |
| 9206 | Physico-chemical study of the complex formation between 2-(tosylamino)benzaldehyde bishydrazones and transition metal ions. <i>Russian Journal of General Chemistry</i> , 2015, 85, 1902-1909. | 0.3 | 2 |
| 9207 | Novel Iminocoumarin Derivatives: Synthesis, Spectroscopic and Computational Studies. <i>Journal of Fluorescence</i> , 2015, 25, 1615-1628. | 1.3 | 18 |
| 9208 | Use of 5-formylfuranboronic acid in the formation of bicyclic boronates with photophysical properties. <i>Inorganica Chimica Acta</i> , 2015, 438, 23-30. | 1.2 | 3 |
| 9209 | Synthesis and structures of monocyclic 1,4-diaza-2,3-diborine species. <i>Inorganic Chemistry Communication</i> , 2015, 61, 214-216. | 1.8 | 9 |
| 9210 | DFT/TD-DFT study of the structural and spectral properties of two forms of Rhodamine B. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550030. | 1.8 | 5 |
| 9211 | Geometry, vibrational frequency, and isomerization of neutral and cation $CuCN$ complex. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550032. | 1.8 | 1 |
| 9212 | Discovering Amorphous Indium Phosphide Nanostructures with High-Temperature ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2015, 119, 23238-23249. | 1.5 | 12 |
| 9213 | A theoretical study of the reaction kinetics of amines released into the atmosphere from CO ₂ capture. <i>International Journal of Greenhouse Gas Control</i> , 2015, 41, 219-228. | 2.3 | 15 |
| 9214 | Depolymerization of Oxidized Lignin Catalyzed by Formic Acid Exploits an Unconventional Elimination Mechanism Involving $3c-4e$ Bonding: A DFT Mechanistic Study. <i>ACS Catalysis</i> , 2015, 5, 6386-6396. | 5.5 | 46 |
| 9215 | Addition reaction of o-carboranyl lithium with nitrile: Formation of a stable zwitterionic iminium salt with a carborane tether. <i>Journal of Organometallic Chemistry</i> , 2015, 799-800, 208-214. | 0.8 | 1 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9216 | Electronic Structure and Absorption Properties of Strongly Coupled Porphyrin-Perylene Arrays. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9879-9888. | 1.1 | 19 |
| 9217 | Visualization of molecular properties at the quantum mechanical level using blender. , 2015, , . | | 3 |
| 9218 | The thermodynamics and biodegradability of chelating agents upon metal extraction. <i>Chemical Engineering Science</i> , 2015, 137, 768-785. | 1.9 | 17 |
| 9219 | Ir(III)-Based Phosphors with Bipyrazolate Ancillaries; Rational Design, Photophysics, and Applications in Organic Light-Emitting Diodes. <i>Inorganic Chemistry</i> , 2015, 54, 10811-10821. | 1.9 | 36 |
| 9220 | A trigonal prismatic Cu ₆ -pyrazolato complex containing a $\frac{1}{4}$ -F ligand. <i>Dalton Transactions</i> , 2015, 44, 20685-20691. | 1.6 | 15 |
| 9221 | A New Approach for Calculating the Band Gap of Semiconductors within the Density Functional Method. <i>Solid State Phenomena</i> , 2015, 242, 434-439. | 0.3 | 2 |
| 9222 | Tension between Internal and External Modes of Stabilization in Carbocations Relevant to Terpene Biosynthesis: Modulating Minima Depth via H \cdots H Interactions. <i>Organic Letters</i> , 2015, 17, 5388-5391. | 2.4 | 22 |
| 9223 | The image charge effect and vibron-assisted processes in Coulomb blockade transport: a first principles approach. <i>Nanoscale</i> , 2015, 7, 19231-19240. | 2.8 | 8 |
| 9224 | A quantum chemical study of unexpected reaction of β -chloroacyl chlorides with 1,2-dichloroethylene in the presence of aluminum chloride. <i>Computational and Theoretical Chemistry</i> , 2015, 1073, 116-122. | 1.1 | 1 |
| 9225 | Electronic Excitations in Solution: The Interplay between State Specific Approaches and a Time-Dependent Density Functional Theory Description. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5782-5790. | 2.3 | 112 |
| 9226 | DFT calculations on polarizabilities and hyperpolarizabilities for the neutral and anionic yttrium oxide clusters. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550049. | 1.8 | 6 |
| 9227 | Structures and absolute stereochemistry of guaiane sesquiterpenoids from the gorgonian <i>Menella woodin</i> . <i>Tetrahedron Letters</i> , 2015, 56, 7001-7004. | 0.7 | 17 |
| 9228 | Ligand Based Dual Fluorescence and Phosphorescence Emission from BODIPY Platinum Complexes and Its Application to Ratiometric Singlet Oxygen Detection. <i>Inorganic Chemistry</i> , 2015, 54, 10946-10957. | 1.9 | 52 |
| 9229 | Mechanism of Manganese-Catalyzed Oxygen Evolution from Experimental and Theoretical Analyses of ¹⁸ O Kinetic Isotope Effects. <i>ACS Catalysis</i> , 2015, 5, 7104-7113. | 5.5 | 41 |
| 9230 | Assessment of the TCA functional in computational chemistry and solid-state physics. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1. | 0.5 | 10 |
| 9231 | Insight into Pd-catalyzed branching cyclizations of enediyne-imides towards furo[2,3-b]pyridines: a DFT study. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 11539-11549. | 1.5 | 9 |
| 9232 | Quantitative Spectra-Structure Relations for Borohydrides. <i>Journal of Physical Chemistry C</i> , 2015, 119, 21868-21874. | 1.5 | 10 |
| 9233 | Two-Step Synthesis of Blue Luminescent (Pyrrolyl)-Heteroaza-indazoles Based on a Three-Component Coupling-Cyclocondensation Sequence. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 5128-5142. | 1.2 | 8 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9234 | Manganese-centered ten-vertex germanium clusters: the strong field Ge ₁₀ ligand encapsulating a transition metal. <i>Journal of Coordination Chemistry</i> , 2015, 68, 3485-3497. | 0.8 | 3 |
| 9235 | Numerical modelling of ion transport in flames. <i>Combustion Theory and Modelling</i> , 2015, 19, 744-772. | 1.0 | 19 |
| 9236 | DFT Investigation of the Mechanism of Action of Organoiridium(III) Complexes As Anticancer Agents. <i>Inorganic Chemistry</i> , 2015, 54, 10801-10810. | 1.9 | 30 |
| 9237 | Computational Studies on Pd-Catalyzed Functionalization of C ₂ H ₂ Using a 1,2,3-Triazole Directing Group: Cyclization versus Substitution. <i>Journal of Organic Chemistry</i> , 2015, 80, 10965-10972. | 1.7 | 4 |
| 9238 | Ab Initio Calculations of Open-Cell Voltage in Li-Ion Organic Radical Batteries. <i>Journal of Physical Chemistry C</i> , 2015, 119, 23373-23378. | 1.5 | 31 |
| 9239 | Importance of Time Scale and Local Environment in Electron-Driven Proton Transfer. The Anion of Acetoacetic Acid. <i>Journal of the American Chemical Society</i> , 2015, 137, 14329-14340. | 6.6 | 11 |
| 9240 | Exploration of charge transfer and absorption spectra of porphyrin-polyoxometalate hybrids to search for high performance sensitizers. <i>RSC Advances</i> , 2015, 5, 93659-93665. | 1.7 | 4 |
| 9241 | Theoretical study on the relative energies of cationic pterin tautomers. <i>Pteridines</i> , 2015, 26, 13-22. | 0.5 | 8 |
| 9242 | Mechanism of the sequential activation of two C-H bonds of a NHC N-methyl group on a triruthenium carbonyl cluster. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1. | 0.5 | 2 |
| 9243 | Ground and excited states of naphthalene-water (naphthalene-W ₆) clusters: a computational study. <i>RSC Advances</i> , 2015, 5, 28281-28291. | 1.7 | 11 |
| 9244 | Quantum Calculations of Electron Tunneling in Respiratory Complex III. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14637-14651. | 1.2 | 8 |
| 9245 | Electronic Structure of Ru ₂ (II,II) Oxypyridinates: Synthetic, Structural, and Theoretical Insights into Axial Ligand Binding. <i>Inorganic Chemistry</i> , 2015, 54, 8571-8589. | 1.9 | 17 |
| 9246 | Key factors in determining the arrangement of Î€-conjugated oligomers inside carbon nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22668-22677. | 1.3 | 12 |
| 9247 | Dual Gold Catalysis: Stepwise Catalyst Transfer via Dinuclear Clusters. <i>Journal of the American Chemical Society</i> , 2015, 137, 10668-10676. | 6.6 | 88 |
| 9248 | An auxiliary-field quantum Monte Carlo study of the chromium dimer. <i>Journal of Chemical Physics</i> , 2015, 142, 064302. | 1.2 | 49 |
| 9249 | The electronic characterization of biphenylene-Experimental and theoretical insights from core and valence level spectroscopy. <i>Journal of Chemical Physics</i> , 2015, 142, 074305. | 1.2 | 24 |
| 9250 | Generic expansion of the Jastrow correlation factor in polynomials satisfying symmetry and cusp conditions. <i>Journal of Chemical Physics</i> , 2015, 142, 084111. | 1.2 | 15 |
| 9251 | H + H ₂ quantum dynamics using potential energy surfaces based on the XYG3 type of doubly hybrid density functionals: Validation of the density functionals. <i>Journal of Chemical Physics</i> , 2015, 142, 084107. | 1.2 | 11 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9252 | Calculating singlet excited states: Comparison with fast time-resolved infrared spectroscopy of coumarins. <i>Journal of Chemical Physics</i> , 2015, 142, 154119. | 1.2 | 14 |
| 9253 | Simulation of circularly polarized luminescence spectra using coupled cluster theory. <i>Journal of Chemical Physics</i> , 2015, 142, 154101. | 1.2 | 26 |
| 9254 | Ensemble density functional theory method correctly describes bond dissociation, excited state electron transfer, and double excitations. <i>Journal of Chemical Physics</i> , 2015, 142, 184104. | 1.2 | 40 |
| 9255 | Communication: Water on hexagonal boron nitride from diffusion Monte Carlo. <i>Journal of Chemical Physics</i> , 2015, 142, 181101. | 1.2 | 56 |
| 9256 | Consistent structures and interactions by density functional theory with small atomic orbital basis sets. <i>Journal of Chemical Physics</i> , 2015, 143, 054107. | 1.2 | 605 |
| 9257 | Prediction of core level binding energies in density functional theory: Rigorous definition of initial and final state contributions and implications on the physical meaning of Kohn-Sham energies. <i>Journal of Chemical Physics</i> , 2015, 142, 214102. | 1.2 | 70 |
| 9258 | Experimental and Theoretical Investigations of Magnetic Exchange Pathways in Structurally Diverse Iron(III) Schiff-Base Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 8625-8638. | 1.9 | 35 |
| 9259 | Toward an Understanding of the Ambiguous Electron Paramagnetic Resonance Spectra of the Iminoxy Radical from <i>o</i> -Fluorobenzaldehyde Oxime: Density Functional Theory and <i>ab Initio</i> Studies. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9109-9120. | 1.1 | 3 |
| 9260 | Co-crystallisation of cytosine with 1,10-phenanthroline: computational screening and experimental realisation. <i>CrystEngComm</i> , 2015, 17, 7130-7141. | 1.3 | 13 |
| 9261 | The growth of phenanthrene from naphthalene by C ₂ H ₂ additions. <i>Molecular Physics</i> , 2015, 113, 1834-1838. | 0.8 | 3 |
| 9262 | Field-induced slow relaxation of magnetization in a pentacoordinate Co(ii) compound [Co(phen)(DMSO)Cl ₂]. <i>Dalton Transactions</i> , 2015, 44, 15014-15021. | 1.6 | 40 |
| 9263 | Different zinc(II) complex species and binding modes at Al^2 N-terminus drive distinct long range cross-talks in the Al^2 monomers. <i>Journal of Inorganic Biochemistry</i> , 2015, 153, 367-376. | 1.5 | 18 |
| 9264 | Charting the known chemical space for non-aqueous lithium-air battery electrolyte solvents. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22596-22603. | 1.3 | 55 |
| 9265 | The interactions between TiO ₂ and graphene with surface inhomogeneity determined using density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29734-29746. | 1.3 | 38 |
| 9266 | Counter-ligand control of the electronic structure in dinuclear copper-tetrakisguanidine complexes. <i>Dalton Transactions</i> , 2015, 44, 19111-19125. | 1.6 | 27 |
| 9267 | Nonvalence Correlation-Bound Anion States of Polycyclic Aromatic Hydrocarbons. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3994-3997. | 2.1 | 21 |
| 9268 | Multireference Character for 4d Transition Metal-Containing Molecules. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5865-5872. | 2.3 | 86 |
| 9269 | Computational and NMR Spectroscopic Evidence for Stereochemistry-Dependent Conformations of 2,2,6,6-Tetramethylpiperidiny-Masked 1,2-Diols. <i>Journal of Organic Chemistry</i> , 2015, 80, 9967-9972. | 1.7 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9270 | Mechanically activated switching of Si-based single-molecule junction as imaged with three-dimensional dynamic probe. <i>Nature Communications</i> , 2015, 6, 8465. | 5.8 | 14 |
| 9271 | Light induced nonlinear optical switch in boronated chromophores: A theoretical search towards high contrast switches in the azobenzene series. <i>Journal of Organometallic Chemistry</i> , 2015, 799-800, 215-222. | 0.8 | 5 |
| 9272 | Enantiodivergent Synthesis of Bis-Spiropyrrolidines via Sequential Interrupted and Completed (3 + 2) Cycloadditions. <i>Journal of Organic Chemistry</i> , 2015, 80, 11755-11767. | 1.7 | 46 |
| 9273 | Long-Range Corrected DFT Meets <i>GW</i> : Vibrationally Resolved Photoelectron Spectra from First Principles. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5391-5400. | 2.3 | 46 |
| 9274 | Structural Properties and UV-Visible Absorption Spectroscopy of Retinal-pyridyl-CN Re(I) Carbonyl Bipyridine Complex: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10645-10653. | 1.1 | 9 |
| 9275 | Structural Characterization of Sm ^{III} (EDTMP). <i>Molecular Pharmaceutics</i> , 2015, 12, 4108-4114. | 2.3 | 8 |
| 9276 | Reaction Intermediates Kinetics in Solution Investigated by Electrospray Ionization Mass Spectrometry: Diaurated Complexes. <i>Journal of the American Chemical Society</i> , 2015, 137, 13647-13657. | 6.6 | 45 |
| 9277 | Unveiling the Atomic-Level Determinants of Acylase-Ligand Complexes: An Experimental and Computational Study. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2227-2241. | 2.5 | 1 |
| 9278 | Charge-Transfer Emission in Organoboron-Based Biphenyls: Effect of Substitution Position and Conformation. <i>Journal of Organic Chemistry</i> , 2015, 80, 10914-10924. | 1.7 | 31 |
| 9279 | Catalytic Formation of Asymmetric Carbodiimides at Mononuclear Chromium(II/IV) Bis(alkoxide) Complexes. <i>Organometallics</i> , 2015, 34, 5119-5128. | 1.1 | 40 |
| 9280 | DFT study of adenine-uracil base pair damage by OH radical. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 645-651. | 0.9 | 6 |
| 9281 | Transition state geometry prediction using molecular group contributions. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 32173-32182. | 1.3 | 42 |
| 9282 | Synthesis, structure and magnetic characterization of dinuclear copper(^{II}) complexes bridged by bicompartamental phenolate. <i>RSC Advances</i> , 2015, 5, 87139-87150. | 1.7 | 32 |
| 9283 | Molecular structure, spectral analysis and hydrogen bonding analysis of ampicillin trihydrate: a combined DFT and AIM approach. <i>New Journal of Chemistry</i> , 2015, 39, 9800-9812. | 1.4 | 53 |
| 9284 | Stochastic Multiconfigurational Self-Consistent Field Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5316-5325. | 2.3 | 86 |
| 9285 | Size-dependent properties of transition metal clusters: from molecules to crystals and surfaces – computational studies with the program ParaGauss. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28463-28483. | 1.3 | 16 |
| 9286 | Chemical trends in the optical properties of rocksalt nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28892-28900. | 1.3 | 10 |
| 9287 | O-H hydrogen bonding promotes H-atom transfer from $\hat{I}\pm$ C-H bonds for C-alkylation of alcohols. <i>Science</i> , 2015, 349, 1532-1536. | 6.0 | 414 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9288 | Semiexperimental Equilibrium Structures for Building Blocks of Organic and Biological Molecules: The B2PLYP Route. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4689-4707. | 2.3 | 95 |
| 9289 | Structure, solvent, and relativistic effects on the NMR chemical shifts in square-planar transition-metal complexes: assessment of DFT approaches. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24944-24955. | 1.3 | 82 |
| 9290 | X-H δ^+ C hydrogen bonds in n-alkane-HX (X = F, OH) complexes are stronger than C-H δ^+ X hydrogen bonds. <i>Journal of Chemical Sciences</i> , 2015, 127, 1035-1045. | 0.7 | 10 |
| 9291 | Synergy of Vicinal Oxygenated Groups of Catalysts for Hydrolysis of Cellulosic Molecules. <i>Journal of Physical Chemistry C</i> , 2015, 119, 20993-20999. | 1.5 | 50 |
| 9292 | DFT as a Powerful Predictive Tool in Photoredox Catalysis: Redox Potentials and Mechanistic Analysis. <i>Organometallics</i> , 2015, 34, 4218-4228. | 1.1 | 57 |
| 9293 | Mechanism of the Intramolecular Hexadehydro-Diels-Alder Reaction. <i>Journal of Organic Chemistry</i> , 2015, 80, 11744-11754. | 1.7 | 49 |
| 9294 | A Quasi-relativistic Density Functional Theory Study of the Actinyl(VI, V) (An = U, Np, Pu) Complexes with a Six-Membered Macrocyclic Containing Pyrrole, Pyridine, and Furan Subunits. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9178-9188. | 1.1 | 35 |
| 9295 | Spherical versus Faceted Anatase TiO ₂ Nanoparticles: A Model Study of Structural and Electronic Properties. <i>Journal of Physical Chemistry C</i> , 2015, 119, 20735-20746. | 1.5 | 58 |
| 9296 | A twist of nature – the significance of atropisomers in biological systems. <i>Natural Product Reports</i> , 2015, 32, 1562-1583. | 5.2 | 420 |
| 9297 | Reactive species involved in the regioselective photooxidation of heptamethine cyanines. <i>Chemical Science</i> , 2015, 6, 6556-6563. | 3.7 | 112 |
| 9298 | Lattice vibration modes of the layered material BiCuSeO and first principles study of its thermoelectric properties. <i>New Journal of Physics</i> , 2015, 17, 083012. | 1.2 | 51 |
| 9299 | Synthesis, spectral, DFT, and semi-empirical study of trimetallic complexes with pyrazole-3,5-dicarboxylic acid containing Sn(IV) and Hg(II). <i>Russian Journal of General Chemistry</i> , 2015, 85, 1725-1733. | 0.3 | 1 |
| 9300 | Reinvestigation of the crystal structure, vibrational spectroscopic studies and DFT calculations of 5-bromo-7-azaindole with dual N-H...N hydrogen bonds in dimers. <i>Journal of Molecular Structure</i> , 2015, 118, 1101, 91-100. | 1.8 | 12 |
| 9301 | Molecular Dynamics Simulations of the Initial-State Predict Product Distributions of Dediazonation of Aryldiazonium in Binary Solvents. <i>Journal of Organic Chemistry</i> , 2015, 80, 8637-8642. | 1.7 | 5 |
| 9302 | Possibility of Copper-Ion-Exchanged MFI-Type Zeolite as C-H Bond Activation Material for Propane and the Driving Force for Activation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 21483-21496. | 1.5 | 12 |
| 9303 | Synthesis, electronic properties, antioxidant and antibacterial activity of some new benzimidazoles. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 6317-6326. | 1.4 | 65 |
| 9304 | Extracting dimer structures from simulations of organic-based materials using QM/MM methods. <i>Chemical Physics</i> , 2015, 459, 112-124. | 0.9 | 4 |
| 9305 | Highly Sensitive Near-Infrared Fluorophores for in Vivo Detection of Amyloid- β^2 Plaques in Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 6972-6983. | 2.9 | 110 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9306 | Interstellar Anions: The Role of Quantum Chemistry. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9941-9953. | 1.1 | 47 |
| 9307 | Dielectric and optical anisotropy enhanced by 1,3-dioxolane terminal substitution on tolane-liquid crystals. <i>Journal of Materials Chemistry C</i> , 2015, 3, 8706-8711. | 2.7 | 48 |
| 9308 | Utilizing fast multipole expansions for efficient and accurate quantum-classical molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2015, 142, 104108. | 1.2 | 5 |
| 9309 | Towards quantifying the role of exact exchange in predictions of transition metal complex properties. <i>Journal of Chemical Physics</i> , 2015, 143, 034104. | 1.2 | 93 |
| 9310 | Calculations of hyperfine coupling constant of copper(II) in aqueous environment. Finite temperature molecular dynamics and relativistic effects. <i>Journal of Molecular Modeling</i> , 2015, 21, 237. | 0.8 | 4 |
| 9311 | Application of reactivity descriptors to the catalytic decomposition of hydrogen peroxide at oxide surfaces. <i>Computational and Theoretical Chemistry</i> , 2015, 1070, 108-116. | 1.1 | 18 |
| 9312 | Acylamido-Based Anion-Functionalized Ionic Liquids for Efficient SO ₂ Capture through Multiple-Site Interactions. <i>ACS Sustainable Chemistry and Engineering</i> , 2015, 3, 2264-2270. | 3.2 | 78 |
| 9313 | Hidden Bond Anomalies: The Peculiar Case of the Fluorinated Amine Chalcogenides. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9541-9556. | 1.1 | 54 |
| 9314 | Multiple-Timestep <i>ab Initio</i> Molecular Dynamics Using an Atomic Basis Set Partitioning. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12119-12130. | 1.1 | 17 |
| 9315 | Ë–extended [12]cycloparaphenylenes: from a hexaphenylbenzene cyclohexamer to its unexpected C ₂ -symmetric congener. <i>Chemical Science</i> , 2015, 6, 7072-7078. | 3.7 | 32 |
| 9316 | The electronic structure of VO in its ground and electronically excited states: A combined matrix isolation and quantum chemical (MRCI) study. <i>Journal of Chemical Physics</i> , 2015, 143, 024309. | 1.2 | 17 |
| 9317 | Rates and Routes of Electron Transfer of [NiFe]-Hydrogenase in an Enzymatic Fuel Cell. <i>Journal of Physical Chemistry B</i> , 2015, 119, 13870-13882. | 1.2 | 11 |
| 9318 | Graphene allotropes under extreme uniaxial strain: an <i>ab initio</i> theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 16418-16427. | 1.3 | 43 |
| 9319 | Relative stabilities of condensed face sharing mono- and di-carboranes: CB ₂₀ H ₁₈ and C ₂ B ₁₉ H ₁₈ ⁺ . <i>Journal of Organometallic Chemistry</i> , 2015, 798, 91-98. | 0.8 | 6 |
| 9320 | Carbon–Nitrogen Bond Construction and Carbon–Oxygen Double Bond Cleavage on a Molecular Titanium Oxonitride: A Combined Experimental and Computational Study. <i>Inorganic Chemistry</i> , 2015, 54, 9401-9412. | 1.9 | 12 |
| 9321 | Four-coordinate nickel(II) and copper(II) complex based ONO tridentate Schiff base ligands: synthesis, molecular structure, electrochemical, linear and nonlinear properties, and computational study. <i>Dalton Transactions</i> , 2015, 44, 18019-18037. | 1.6 | 62 |
| 9322 | Computational thermodynamic study on the complexes of Am(III) with tridentate N-donor ligands. <i>New Journal of Chemistry</i> , 2015, 39, 7716-7729. | 1.4 | 9 |
| 9323 | Synthesis and energetic properties of high-nitrogen substituted bishomocubanes. <i>Journal of Materials Chemistry A</i> , 2015, 3, 22118-22128. | 5.2 | 29 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9324 | Raman scattering studies of order parameters in liquid crystalline dimers exhibiting the nematic and twist-bend nematic phases. <i>Journal of Materials Chemistry C</i> , 2015, 3, 10007-10016. | 2.7 | 71 |
| 9325 | The reactivity of stoichiometric tungsten oxide clusters towards carbon monoxide: the effects of cluster sizes and charge states. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11499-11508. | 1.3 | 7 |
| 9326 | N-2-Aryl-1,2,3-Triazoles: A novel class of blue-green emitting fluorophores-synthesis, photophysical properties study and dft computations. <i>Journal of Luminescence</i> , 2015, 168, 114-123. | 1.5 | 9 |
| 9327 | An evaluation of indirubin analogues as phosphorylase kinase inhibitors. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 61, 231-242. | 1.3 | 11 |
| 9328 | A structural study of LiTFSI-tetraglyme mixtures: From diluted solutions to solvated ionic liquids. <i>Journal of Molecular Liquids</i> , 2015, 210, 238-242. | 2.3 | 62 |
| 9329 | TOWARD THE FORMATION OF CARBONACEOUS REFRACTORY MATTER IN HIGH TEMPERATURE HYDROCARBON-RICH ATMOSPHERES OF EXOPLANETS UPON MICROMETEOROID IMPACT. <i>Astrophysical Journal</i> , 2015, 805, 76. | 1.6 | 24 |
| 9330 | Assessing Molecular Dynamics Simulations with Solvatochromism Modeling. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10693-10700. | 1.2 | 15 |
| 9331 | C ⁺ Cyclometalated Platinum(II) Complexes with Dibenzofuranyl-1,2,4-triazol-5-ylidene Ligands: Synthesis, Characterization, and Photoluminescent Properties. <i>Organometallics</i> , 2015, 34, 4433-4440. | 1.1 | 20 |
| 9332 | Halogen Photoelimination from Monomeric Nickel(III) Complexes Enabled by the Secondary Coordination Sphere. <i>Organometallics</i> , 2015, 34, 4766-4774. | 1.1 | 73 |
| 9333 | The energetic viability of an unexpected skeletal rearrangement in cyclooctatin biosynthesis. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 10273-10278. | 1.5 | 40 |
| 9334 | Simulating Cl K-edge X-ray absorption spectroscopy in MCl ₆ ²⁻ (M = U, Np, Pu) complexes and UOCl ₅ - using time-dependent density functional theory. <i>Highlights in Theoretical Chemistry</i> , 2015, , 247-253. | 0.0 | 2 |
| 9335 | Predicting hydration propensities of biologically relevant α -ketoamides. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015, 25, 4153-4157. | 1.0 | 5 |
| 9336 | A systematic benchmark of the <i>ab initio</i> Bethe-Salpeter equation approach for low-lying optical excitations of small organic molecules. <i>Journal of Chemical Physics</i> , 2015, 142, 244101. | 1.2 | 137 |
| 9337 | Density-matrix based determination of low-energy model Hamiltonians from <i>ab initio</i> wavefunctions. <i>Journal of Chemical Physics</i> , 2015, 143, 102814. | 1.2 | 23 |
| 9338 | Aromaticity Induced by Electric Field: The Case of Polycalicyenes. <i>Journal of Organic Chemistry</i> , 2015, 80, 9091-9101. | 1.7 | 4 |
| 9339 | Catalytic Role of the Substrate Defines Specificity of Therapeutic L-Asparaginase. <i>Journal of Molecular Biology</i> , 2015, 427, 2867-2885. | 2.0 | 25 |
| 9340 | Azo-based iminopyridine ligands: synthesis, optical properties, theoretical calculations and complexation studies. <i>Tetrahedron</i> , 2015, 71, 7911-7919. | 1.0 | 12 |
| 9341 | Azo dicarboxylates are not conjugated: X-ray crystal structure and theoretical calculations on di- <i>t</i> -butylazodicarboxylate. <i>Journal of Molecular Structure</i> , 2015, 1098, 298-305. | 1.8 | 4 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9342 | Experimental and Theoretical Investigations of the Bromination of Phenols with \hat{I}^2 and \hat{I}^3 Aliphatic Substituents, including Rings. <i>Journal of Organic Chemistry</i> , 2015, 80, 9292-9296. | 1.7 | 1 |
| 9343 | Counterion influence on the Nâ€“Iâ€“N halogen bond. <i>Chemical Science</i> , 2015, 6, 3746-3756. | 3.7 | 100 |
| 9344 | 2,5-Bridged 1-Carba- <i>arachno</i> -pentaborane(10) Derivatives â€“ Intermediates on the Way to Pentaalkyl-1,5-dicarb- <i>closo</i> -pentaboranes(5). <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2015, 70, 741-745. | 0.3 | 2 |
| 9346 | Exploring the MP2 energy surface of nanoalloy clusters with a genetic algorithm: Application to sodiumâ€“potassium. <i>Chemical Physics Letters</i> , 2015, 639, 135-141. | 1.2 | 15 |
| 9347 | Structural and Vibrational Spectroscopic Analysis of Anticancer Drug Mitotane Using Density Functional Theory. <i>Materials Today: Proceedings</i> , 2015, 2, 965-968. | 0.9 | 2 |
| 9348 | Structural Properties of Green Tea Catechins. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12860-12867. | 1.2 | 93 |
| 9349 | Enhanced multiple exciton generation in amorphous silicon nanowires and films. <i>Molecular Physics</i> , 0, , 1-15. | 0.8 | 7 |
| 9350 | The effect of fluorine substitution on the conformation and aromaticity of \hat{I} -6-fluoro arene chromium tricarbonyl complexes â€“ Density functional insights. <i>Computational and Theoretical Chemistry</i> , 2015, 1069, 125-131. | 1.1 | 11 |
| 9351 | Reactivity of Dimeric Tetrazirconium(IV) Wellsâ€“Dawson Polyoxometalate toward Dipeptide Hydrolysis Studied by a Combined Experimental and Density Functional Theory Approach. <i>Inorganic Chemistry</i> , 2015, 54, 11477-11492. | 1.9 | 32 |
| 9352 | Synthesis, Crystal Structure, Physical Properties and Theoretical Calculations of a New One-Dimensional Ni(II) Coordination Polymer Constructed by 1,10-Phenanthroline Derivative Ligand and Sulfate. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2015, 25, 1441-1447. | 1.9 | 3 |
| 9353 | Binuclear sandwich and multi-decker sandwich compounds of alkali and alkaline-earth metals: a quantum chemical study. <i>Russian Chemical Bulletin</i> , 2015, 64, 540-550. | 0.4 | 3 |
| 9354 | Spectroscopic and structural analysis of mixed carbon dioxide and fluorinated methane clusters. <i>Chemical Physics Letters</i> , 2015, 638, 191-195. | 1.2 | 8 |
| 9355 | The impact of particle size on the adsorption of citrate to hematite. <i>Journal of Colloid and Interface Science</i> , 2015, 460, 36-46. | 5.0 | 32 |
| 9356 | Enhanced Raman scattering from aromatic dithiols electrospayed into plasmonic nanojunctions. <i>Faraday Discussions</i> , 2015, 184, 339-357. | 1.6 | 15 |
| 9357 | Prediction of the Standard Gibbs Energy of Transfer of Organic Ions Across the Interface between Two Immiscible Liquids. <i>Journal of Physical Chemistry B</i> , 2015, 119, 13167-13176. | 1.2 | 16 |
| 9358 | Electronic Structure of Fullerene Acceptors in Organic Bulk-Heterojunctions: A Combined EPR and DFT Study. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4730-4735. | 2.1 | 14 |
| 9359 | Inter-Excited-State Phosphorescence in the Four-Component Relativistic Kohnâ€“Sham Approximation: A Case Study on Lumiflavin. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11911-11921. | 1.1 | 7 |
| 9360 | Systematic Assessment of the Photochemical Stability of Photoinitiator-Derived Macromolecular Chain Termini. <i>Macromolecules</i> , 2015, 48, 8451-8460. | 2.2 | 12 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9361 | Importance of the Electron Correlation and Dispersion Corrections in Calculations Involving Enamines, Hemiaminals, and Aminals. Comparison of B3LYP, M06-2X, MP2, and CCSD Results with Experimental Data. <i>Journal of Organic Chemistry</i> , 2015, 80, 11977-11985. | 1.7 | 27 |
| 9362 | Experimental and theoretical studies of triisopropanolamine as an inhibitor for aluminum alloy in 3% NaCl solution. <i>RSC Advances</i> , 2015, 5, 101693-101700. | 1.7 | 25 |
| 9363 | Simulating Valence-to-Core X-ray Emission Spectroscopy of Transition Metal Complexes with Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5804-5809. | 2.3 | 49 |
| 9364 | Anharmonic Vibrational Treatment Exclusively in Curvilinear Valence Coordinates: The Case of Formamide. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11719-11728. | 1.1 | 8 |
| 9365 | Activity prediction of substrates in NADH-dependent carbonyl reductase by docking requires catalytic constraints and charge parameterization of catalytic zinc environment. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 1057-1069. | 1.3 | 17 |
| 9366 | Reaction of Copper(II) Chloroacetate with Pyrazole. Synthesis of a One-Dimensional Coordination Polymer and Unexpected Dehydrochlorination Reaction. <i>Crystal Growth and Design</i> , 2015, 15, 5910-5918. | 1.4 | 18 |
| 9367 | Effect of π - π interaction in Bergman cyclisation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29793-29802. | 1.3 | 3 |
| 9368 | XMVB 2.0: A new version of Xiamen valence bond program. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 731-737. | 1.0 | 65 |
| 9369 | Multiconfiguration Pair-Density Functional Theory: Barrier Heights and Main Group and Transition Metal Energetics. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 82-90. | 2.3 | 62 |
| 9370 | Theoretical Investigation on Rhodium(I)-Catalyzed Cycloisomerizations of 4-Allenal Species with Linked Alkyne: Ketone vs Alcohol Products. <i>Organometallics</i> , 2015, 34, 280-288. | 1.1 | 9 |
| 9371 | Mechanism of Redox-Active Ligand-Assisted Nitrene-Group Transfer in a Zr ^{IV} Complex: Direct Ligand-to-Ligand Charge Transfer Preferred. <i>Chemistry - A European Journal</i> , 2015, 21, 1780-1789. | 1.7 | 9 |
| 9372 | The mechanism of Cu-catalyzed C ⁼ N cyclization from N-phenylbenzamidine to 2-phenylbenzimidazole: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2015, 1054, 16-21. | 1.1 | 13 |
| 9373 | The CH ₃ CHOO ⁻ Criegee intermediate TM and its anion: Isomers, infrared spectra, and W3-F12 energetics. <i>Chemical Physics Letters</i> , 2015, 621, 193-198. | 1.2 | 6 |
| 9374 | Toward the construction of parameter-free doubly hybrid density functionals. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 589-595. | 1.0 | 22 |
| 9375 | ³ He NMR studies on helium-pyrrole, helium-indole, and helium-carbazole systems: a new tool for following chemistry of heterocyclic compounds. <i>Magnetic Resonance in Chemistry</i> , 2015, 53, 103-109. | 1.1 | 9 |
| 9376 | Nonafluorobutanesulfonyl Azide as a Shelf-Stable Highly Reactive Oxidant for the Copper-Catalyzed Synthesis of 1,3-Diynes from Terminal Alkynes. <i>Journal of Organic Chemistry</i> , 2015, 80, 1098-1106. | 1.7 | 24 |
| 9377 | Experimental and Computational Study of the Catalytic Asymmetric 4 π -Electrocyclization of N α -Heterocycles. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 2762-2765. | 7.2 | 50 |
| 9378 | Synthesis of two nickel (II) complexes bearing pyrrolide-imine ligand and their catalytic effects on thermal decomposition of ammonium perchlorate. <i>Journal of Molecular Structure</i> , 2015, 1085, 13-20. | 1.8 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9379 | Theoretical studies on POM-based organic-inorganic hybrids containing double D _{3h} -A _{1g} -A _{2g} chains for high-performance p-type, dye-sensitized solar cells (DSSCs). <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5459-5465. | 1.3 | 31 |
| 9380 | Rhenabenzenes and Unexpected Coupling Products from the Reactions of Rhenacyclobutadienes with Ethoxyethyne. <i>Organometallics</i> , 2015, 34, 167-176. | 1.1 | 27 |
| 9381 | Tuning Proton Conductivity in Alkali Metal Phosphonocarboxylates by Cation Size-Induced and Water-Facilitated Proton Transfer Pathways. <i>Chemistry of Materials</i> , 2015, 27, 424-435. | 3.2 | 82 |
| 9382 | Calculation of the vibrational frequencies of carbon clusters and fullerenes with empirical potentials. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 3898-3908. | 1.3 | 12 |
| 9383 | Normal co-ordinate analysis, molecular structural, non-linear optical, second order perturbation studies of Tizanidine by density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 139, 189-199. | 2.0 | 2 |
| 9384 | The Chemical Electronic Properties of PNP Molecular Transistor Based on (4,3) Chiral Carbon Nanotube. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2015, 23, 218-232. | 1.0 | 1 |
| 9385 | Protein-Like Dynamics of Polycarbonate Polymers in Water. <i>Journal of Physical Chemistry B</i> , 2015, 119, 316-329. | 1.2 | 5 |
| 9386 | Click chemistry mediated synthesis of bio-inspired phosphonyl-functionalized ionic liquids. <i>Green Chemistry</i> , 2015, 17, 1259-1268. | 4.6 | 12 |
| 9387 | Directed Metalation of 1-Ester-Substituted Indolizines: Base/Electrophile-Controlled Regioselective Functionalization. <i>Organic Letters</i> , 2015, 17, 238-241. | 2.4 | 39 |
| 9388 | Quantum Chemical Interpretation of Ultrafast Luminescence Decay and Intersystem Crossings in Rhenium(I) Carbonyl Bipyridine Complexes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 99-110. | 2.3 | 39 |
| 9389 | Quantum mechanical and experimental analyses of TNT metabolite 2-hydroxylamino-4,6-dinitrotoluene. <i>Journal of Molecular Structure</i> , 2015, 1080, 145-152. | 1.8 | 4 |
| 9390 | Halogen bonding in the antibacterial 1,2,4-triazole-3-thione derivative - Spectroscopic properties, crystal structure and conformational analysis. <i>Journal of Molecular Structure</i> , 2015, 1083, 187-193. | 1.8 | 14 |
| 9391 | An assessment of theoretical procedures for π -conjugation stabilisation energies in enones. <i>Molecular Physics</i> , 2015, 113, 1284-1296. | 0.8 | 19 |
| 9392 | Facile diastereoselective synthesis of cis-perfluoroalkylated fused [1,3]oxazines from aromatic aldehydes, methyl perfluoroalk-2-ynoates and quinolines. <i>Tetrahedron</i> , 2015, 71, 622-629. | 1.0 | 13 |
| 9393 | Ligand-Sensitive But Not Ligand-Diagnostic: Evaluating Cr Valence-to-Core X-ray Emission Spectroscopy as a Probe of Inner-Sphere Coordination. <i>Inorganic Chemistry</i> , 2015, 54, 205-214. | 1.9 | 32 |
| 9394 | Mechanisms of the hydroxyl and superoxide anion radical scavenging activity and protective effect on lipid peroxidation of thymoquinone: a DFT study. <i>Monatshefte für Chemie</i> , 2015, 146, 601-611. | 0.9 | 13 |
| 9395 | Computational Analysis of the Stereochemical Outcome in the Imidazolidinone-Catalyzed Enantioselective (4 + 3)-Cycloaddition Reaction. <i>Journal of Organic Chemistry</i> , 2015, 80, 744-750. | 1.7 | 26 |
| 9396 | 11,11-Dimethyl-1,6-methano[10]annulene - An Annulene with an Ultralong CC Bond or a Fluxional Molecule?. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1666-1682. | 1.1 | 41 |

| # | ARTICLE | IF | CITATIONS |
|------|--|------|-----------|
| 9397 | Quantum chemical calculations and interpretation of electronic transitions and spectroscopic characteristics belonging to 1-(3-Mesityl-3-methylcyclobutyl)-2-(naphthalene-1-yloxy)ethanone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 899-912. | 2.0 | 0 |
| 9398 | Sulphur-bearing species in molecular clouds. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015, 446, 3118-3129. | 1.6 | 13 |
| 9399 | Analysis of computational models for an accurate study of electronic excitations in GFP. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2582-2588. | 1.3 | 47 |
| 9400 | Structure of Plasma Poly(Acrylic Acid): Influence of Pressure and Dielectric Properties. <i>Plasma Chemistry and Plasma Processing</i> , 2015, 35, 303-320. | 1.1 | 20 |
| 9401 | Effect of methoxy group instead of polar group in the nematic phase of four-ring bent-core liquid crystals. <i>RSC Advances</i> , 2015, 5, 7001-7006. | 1.7 | 14 |
| 9402 | Synthesis and optical properties of a D ⁺ A ⁻ D cationic cyclopentadienyl iron complex containing double arylazo chromophores. <i>Research on Chemical Intermediates</i> , 2015, 41, 8245-8255. | 1.3 | 0 |
| 9403 | <sc>HONPAS</sc>: A linear scaling open-source solution for large system simulations. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 647-655. | 1.0 | 34 |
| 9404 | Selective complexation of alkaline earth metal ions with nanotubular cyclopeptides: DFT theoretical study. <i>RSC Advances</i> , 2015, 5, 2305-2317. | 1.7 | 23 |
| 9405 | Excited States of Ladder-Type π -Conjugated Dyes with a Joint SOS-CIS(D) and PCM-TD-DFT Approach. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5417-5425. | 1.1 | 13 |
| 9406 | Protocols Utilizing Constant pH Molecular Dynamics to Compute pH-Dependent Binding Free Energies. <i>Journal of Physical Chemistry B</i> , 2015, 119, 861-872. | 1.2 | 29 |
| 9407 | Effect of Stacking Interactions on the Thermodynamics and Kinetics of Lumiflavin: A Study with Improved Density Functionals and Density Functional Tight-Binding Protocol. <i>Journal of Physical Chemistry A</i> , 2015, 119, 172-182. | 1.1 | 13 |
| 9408 | Thermochemistry of Halogen-Substituted Methylbenzenes. <i>Journal of Chemical & Engineering Data</i> , 2015, 60, 89-103. | 1.0 | 170 |
| 9409 | Palladium-Catalyzed Enantioselective Decarboxylative Cycloaddition of Vinyl ethylene Carbonates with Isocyanates. <i>Chemistry - A European Journal</i> , 2015, 21, 120-124. | 1.7 | 111 |
| 9410 | Oxidation-induced water-solubilization and chemical functionalization of fullerenes C ₆₀ , Gd@C ₆₀ and Gd@C ₈₂ : atomistic insights into the formation mechanisms and structures of fullereneols synthesized by different methods. <i>Nanoscale</i> , 2015, 7, 2914-2925. | 2.8 | 27 |
| 9411 | Highly efficient blue electroluminescence based on thermally activated delayed fluorescence. <i>Nature Materials</i> , 2015, 14, 330-336. | 13.3 | 1,129 |
| 9412 | Structural and theoretical studies on rhodium and iridium complexes with 5-nitrosopyrimidines. Effects on the proteolytic regulatory enzymes of the renin-angiotensin system in human tumoral brain cells. <i>Journal of Inorganic Biochemistry</i> , 2015, 143, 20-33. | 1.5 | 12 |
| 9413 | Theoretical study and design of multifunctional phosphorescent platinum(<i>ii</i>) complexes containing triarylboron moieties for efficient OLED emitters. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2438-2446. | 1.3 | 30 |
| 9414 | Electrochemical sensors using gold submicron particles modified electrodes based on calcium complexes formed with alizarin red S for determination of Ca ²⁺ in isolated rat heart mitochondria. <i>Biosensors and Bioelectronics</i> , 2015, 66, 417-422. | 5.3 | 14 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9415 | Novel uranyl(ν) complexes incorporating propylene-bridged salen-type N_2O_2 -ligands: a structural and computational approach. Dalton Transactions, 2015, 44, 568-577. | 1.6 | 40 |
| 9416 | Using dispersion-corrected density functional theory to understand supramolecular binding thermodynamics. Chemical Communications, 2015, 51, 1764-1774. | 2.2 | 125 |
| 9417 | Visualizing phosphodiester-bond hydrolysis by an endonuclease. Nature Structural and Molecular Biology, 2015, 22, 65-72. | 3.6 | 30 |
| 9418 | Influence of the Density Functional and Basis Set on the Relative Stabilities of Oxygenated Isomers of Diiron Models for the Active Site of [FeFe]-Hydrogenase. Journal of Chemical Theory and Computation, 2015, 11, 205-214. | 2.3 | 13 |
| 9419 | Photoinduced Proton Transfer Promoted by Peripheral Subunits for Some Hantzsch Esters. Journal of Physical Chemistry A, 2015, 119, 39-49. | 1.1 | 9 |
| 9420 | Improving the $Q2MM$ method for transition state force field modeling. Journal of Computational Chemistry, 2015, 36, 244-250. | 1.5 | 9 |
| 9421 | Structural characterization of unusually stable polycyclic ozonides. Journal of Molecular Structure, 2015, 1082, 151-161. | 1.8 | 2 |
| 9422 | Segmented Contracted Basis Sets Optimized for Nuclear Magnetic Shielding. Journal of Chemical Theory and Computation, 2015, 11, 132-138. | 2.3 | 235 |
| 9423 | Theoretical study of the mechanism of protein arginine deiminase 4 (PAD4) inhibition by F-amidine. Journal of Molecular Graphics and Modelling, 2015, 55, 25-32. | 1.3 | 10 |
| 9424 | Ring- and side-group conformational properties of di-O-acylated xylopyranosides: A computational study. Computational and Theoretical Chemistry, 2015, 1051, 104-109. | 1.1 | 2 |
| 9425 | Charge transfer dynamics from adsorbates to surfaces with single active electron and configuration interaction based approaches. Chemical Physics, 2015, 446, 24-29. | 0.9 | 7 |
| 9426 | Structural, spectroscopic and theoretical studies of dimethylphenyl betaine complex with two molecules of 2,6-dichloro-4-nitro-phenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1216-1226. | 2.0 | 10 |
| 9427 | Structure, stability, energy barrier and ionization energies of chemically modified DNA-bases: Quantum chemical calculations on 37 favored and rare tautomeric forms of tetraphosphoadenine. Computational and Theoretical Chemistry, 2015, 1052, 35-41. | 1.1 | 4 |
| 9428 | Magnetic and structural properties of dinuclear singly bridged-phenoxido metal(ν) complexes. Dalton Transactions, 2015, 44, 2110-2121. | 1.6 | 39 |
| 9429 | The selectivity of diglycolamide (TODGA) and bis-triazine-bipyridine (BTBP) ligands in actinide/lanthanide complexation and solvent extraction separation \hat{a} €“ a theoretical approach. Dalton Transactions, 2015, 44, 2657-2666. | 1.6 | 91 |
| 9430 | Ionic Ferrocenyl Compounds Containing Polycyano Anions. Synthesis, Structures, and Effects on Thermal Decomposition of Core Components of Solid Propellants. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2015, 641, 475-482. | 0.6 | 14 |
| 9431 | Theoretical study on reaction mechanism of an N-heterocyclic carbene boryl azide with electron-deficient alkynes and nitriles. Structural Chemistry, 2015, 26, 599-606. | 1.0 | 4 |
| 9432 | Simultaneous generation of mild acidic functionalities and small supported Ir NPs from alumina-supported well-defined iridium siloxide. Journal of Catalysis, 2015, 321, 81-89. | 3.1 | 24 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9433 | In search of molecular scale devices: Theoretical study of linearly fused straight single-walled carbon nanotube junctions based on the pentagon/heptagon pair defects. <i>Computational Materials Science</i> , 2015, 98, 201-210. | 1.4 | 5 |
| 9434 | Biomimetic One-Pot Route to Acridine Epoxides. <i>Journal of Organic Chemistry</i> , 2015, 80, 281-289. | 1.7 | 16 |
| 9435 | Experimental and Theoretical Approaches to the Influence of the Addition of Pyrene to a Series of Pd and Ni NHC-Based Complexes: Catalytic Consequences. <i>Chemistry - A European Journal</i> , 2015, 21, 1578-1588. | 1.7 | 44 |
| 9436 | Virtual Eyes Designed for Quantitative Spectroscopy of Inorganic Complexes: Vibronic Signatures in the Phosphorescence Spectra of Terpyridine Derivatives. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7253-7257. | 1.2 | 17 |
| 9437 | Evaluating the accuracy of density functional theory for calculating ¹ H and ¹³ C NMR chemical shifts in drug molecules. <i>Computational and Theoretical Chemistry</i> , 2015, 1051, 161-172. | 1.1 | 18 |
| 9438 | DFT calculations and experimental FT-IR, FT-Raman, NMR, UV-Vis spectral studies of 3-fluorophenylboronic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 306-320. | 2.0 | 33 |
| 9439 | Water-mediated interactions between trimethylamine-N-oxide and urea. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 298-306. | 1.3 | 70 |
| 9440 | Identifying dominant conformations of N-acetyl-L-cysteine methyl ester and N-acetyl-L-cysteine in water: VCD signatures of the amide I and the CO stretching bands. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 131-140. | 2.0 | 8 |
| 9441 | (C ¹³)-cyclometalated platinum(II) imidazo[1,5-a]pyridine NHC complexes – Synthesis and characterization. <i>Journal of Organometallic Chemistry</i> , 2015, 775, 155-163. | 0.8 | 18 |
| 9442 | Vibrations and reorientations of NH ₃ molecules in [Mn(NH ₃) ₆](ClO ₄) ₂ studied by infrared spectroscopy and theoretical (DFT) calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1515-1522. | 2.0 | 10 |
| 9443 | X-ray crystal structure, vibrational spectra and DFT calculations of 3-chloro-7-azaindole: A case of dual N-H...N hydrogen bonds in dimers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 405-415. | 2.0 | 12 |
| 9444 | Fragmentation pathways analysis for the gas phase dissociation of protonated carnosine-oxaliplatin complexes. <i>Dalton Transactions</i> , 2015, 44, 4455-4467. | 1.6 | 6 |
| 9445 | Automatic GROMACS Topology Generation and Comparisons of Force Fields for Solvation Free Energy Calculations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 810-823. | 1.2 | 88 |
| 9446 | A computational view on the reactions of hydrocarbons with coinage metal complexes. <i>Journal of Organometallic Chemistry</i> , 2015, 784, 2-12. | 0.8 | 39 |
| 9447 | Efficiency phosphorescent OLEDs with a low roll-off based on a hetero-triplet iridium complex. <i>Dyes and Pigments</i> , 2015, 113, 649-654. | 2.0 | 15 |
| 9448 | Linearity condition for orbital energies in density functional theory (V): Extension to excited state calculations. <i>Chemical Physics Letters</i> , 2015, 618, 30-36. | 1.2 | 5 |
| 9449 | Identification of novel tyrosine kinase inhibitors for drug resistant T315I mutant BCR-ABL: a virtual screening and molecular dynamics simulations study. <i>Scientific Reports</i> , 2014, 4, 6948. | 1.6 | 59 |
| 9450 | Mechanistic Study of the Titanocene(III)-Catalyzed Radical Arylation of Epoxides. <i>Chemistry - A European Journal</i> , 2015, 21, 280-289. | 1.7 | 71 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9451 | Dâ€“â€“A Triarylboron Compounds with Tunable Pushâ€“Pull Character Achieved by Modification of Both the Donor and Acceptor Moieties. <i>Chemistry - A European Journal</i> , 2015, 21, 177-190. | 1.7 | 125 |
| 9452 | Application of quantum calculations in the chemical industryâ€“An overview. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 107-136. | 1.0 | 74 |
| 9453 | Calculating accurate barriers for olefin insertion and related reactions. <i>Journal of Organometallic Chemistry</i> , 2015, 775, 39-49. | 0.8 | 56 |
| 9454 | Phosphorus as a heteroatom in metallaborane structures: Cyclopentadienylcobalt diphosphaboranes. <i>Polyhedron</i> , 2015, 85, 933-940. | 1.0 | 5 |
| 9455 | LDA+U/GGA+U calculations of structural and electronic properties of CdTe: Dependence on the effective U parameter. <i>Computational Materials Science</i> , 2015, 98, 18-23. | 1.4 | 25 |
| 9456 | A Simple Method for Estimating the Absolute Solvation Free Energy of Monovalent Ions in Different Solvents. <i>Journal of Physical Chemistry A</i> , 2015, 119, 160-171. | 1.1 | 5 |
| 9457 | Synthesis and the absolute configuration of both enantiomers of 4,5-dihydroxy-3-(formyl)cyclopent-2-enone acetonide as a new chiral building block for prostanoid synthesis. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 807-816. | 1.5 | 7 |
| 9458 | In search of an intrinsic chemical bond. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 31-37. | 1.1 | 28 |
| 9459 | Phenylazoindole dyes 3: Determination of azo-hydrazone tautomers of new phenylazoindole dyes in solution and solid state. <i>Journal of Molecular Structure</i> , 2015, 1081, 175-181. | 1.8 | 25 |
| 9460 | Molecular Structure of 1,2-Bis(trifluoromethyl)-1,1,2,2-tetramethyldisilane in the Gas, Liquid, and Solid Phases: Unusual Conformational Changes between Phases. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1600-1608. | 1.1 | 3 |
| 9461 | Computing pK_a values of hexaâ€“aqua transition metal complexes. <i>Journal of Computational Chemistry</i> , 2015, 36, 69-78. | 1.5 | 26 |
| 9462 | Gas-phase thermochemical properties of some tri-substituted phenols: A density functional theory study. <i>Journal of Chemical Thermodynamics</i> , 2015, 80, 65-72. | 1.0 | 5 |
| 9463 | Mechanism of the addition of alkynes to silenes and germenenes: A density functional study. <i>Canadian Journal of Chemistry</i> , 2015, 93, 134-142. | 0.6 | 12 |
| 9464 | Structural and spectroscopic investigation of the N-methylformamideâ€“water (NMFâ€“ $3H_2O$) complex. <i>Molecular Physics</i> , 2015, 113, 149-159. | 0.8 | 2 |
| 9465 | A TDDFT/EFP1 study on hydrogen bonding dynamics of coumarin 151 in water. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 99-104. | 2.0 | 9 |
| 9466 | Molecular Orbital Based Design Guideline for Hypergolic Ionic Liquids. <i>Propellants, Explosives, Pyrotechnics</i> , 2015, 40, 144-149. | 1.0 | 15 |
| 9467 | Thermochemistry of 1-alkylimidazoles. <i>Journal of Chemical Thermodynamics</i> , 2015, 80, 59-64. | 1.0 | 7 |
| 9468 | Spectrophotometric, voltammetric and cytotoxicity studies of 2-hydroxy-5-methoxyacetophenone thiosemicarbazone and its N(4)-substituted derivatives: A combined experimentalâ€“computational study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 719-725. | 2.0 | 9 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9469 | Synthesis and optical properties of two cationic cyclopentadienyliron complexes of arene containing the triphenylbutene structure. <i>Research on Chemical Intermediates</i> , 2015, 41, 5095-5108. | 1.3 | 2 |
| 9470 | Molecular structure, vibrational spectral assignments, HOMO–LUMO, MESP, Mulliken analysis and thermodynamic properties of 2,6-xyleneol and 2,5-dimethyl cyclohexanol based on DFT calculation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 490-502. | 2.0 | 24 |
| 9471 | The crystal structure of sulfamethoxazole, interaction with DNA, DFT calculation, and molecular docking studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 560-568. | 2.0 | 20 |
| 9472 | Redox transformations in electroactive polymer films derived from complexes of nickel with SalEn-type ligands: computational, EQCM, and spectroelectrochemical study. <i>Journal of Solid State Electrochemistry</i> , 2015, 19, 453-468. | 1.2 | 36 |
| 9473 | Synthesis and characterization of an insoluble polymer based on polyamidoamine: Applications for the decontamination of metals in aqueous systems. <i>Journal of Environmental Management</i> , 2015, 147, 321-329. | 3.8 | 10 |
| 9474 | Carbazole-bridged double dye for efficient dye-sensitized solar cell. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2015, 296, 1-10. | 2.0 | 15 |
| 9475 | Guaiane Sesquiterpenoids from the Gorgonian <i>Menella woodin</i> . <i>Natural Product Communications</i> , 2016, 11, 1934578X1601100. | 0.2 | 2 |
| 9476 | Methylpalladium complexes with pyrimidine-functionalized N-heterocyclic carbene ligands. <i>Beilstein Journal of Organic Chemistry</i> , 2016, 12, 1557-1565. | 1.3 | 3 |
| 9477 | Characterization of the synthetic cannabinoid MDMB-CHMCZCA. <i>Beilstein Journal of Organic Chemistry</i> , 2016, 12, 2808-2815. | 1.3 | 21 |
| 9478 | Ring-whizzing in polyene-PtL ₂ complexes revisited. <i>Beilstein Journal of Organic Chemistry</i> , 2016, 12, 1410-1420. | 1.3 | 2 |
| 9479 | Alternative bridging architectures in organic nonlinear optical materials: comparison of π - and π -type structures. <i>Journal of the Optical Society of America B: Optical Physics</i> , 2016, 33, E160. | 0.9 | 3 |
| 9480 | Theoretical Studies on Hydrogen Bonds in Anions Encapsulated by an Azamacrocyclic Receptor. <i>Crystals</i> , 2016, 6, 31. | 1.0 | 2 |
| 9481 | The hydrolysis of geminal ethers: a kinetic appraisal of orthoesters and ketals. <i>Beilstein Journal of Organic Chemistry</i> , 2016, 12, 1467-1475. | 1.3 | 7 |
| 9482 | Theoretical Investigation of Mono- and Di-Chloro-Substituent Effects on the Insulation and Greenhouse Properties of Octafluorocyclobutane. <i>Frontiers in Chemistry</i> , 2016, 4, 47. | 1.8 | 0 |
| 9483 | Theoretical Studies on Electrophilic Aromatic Substitution Reaction for 8-Hydroxyquinoline. <i>Oriental Journal of Chemistry</i> , 2016, 32, 253-260. | 0.1 | 2 |
| 9484 | Influence of the Localization of Ge Atoms within the Si(001)(4 Å–2) Surface Layer on Semicore One-Electron States. <i>Computation</i> , 2016, 4, 14. | 1.0 | 1 |
| 9485 | Hexakis (propargyl-1H-tetrazole) Iron(II) X ₂ [X = BF ₄ , ClO ₄]—Spin Switchable Complexes with Functionalization Potential and the Myth of the Explosive SCO Compound. <i>Magnetochemistry</i> , 2016, 2, 12. | 1.0 | 9 |
| 9486 | Towards Water Soluble Mitochondria-Targeting Theranostic Osmium(II) Triazole-Based Complexes. <i>Molecules</i> , 2016, 21, 1382. | 1.7 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9487 | Pentacoordinate and Hexacoordinate Mn(III) Complexes of Tetradentate Schiff-Base Ligands Containing Tetracyanidoplatinate(II) Bridges and Revealing Uniaxial Magnetic Anisotropy. <i>Molecules</i> , 2016, 21, 1681. | 1.7 | 13 |
| 9488 | Fluoride Anion Recognition by a Multifunctional Urea Derivative: An Experimental and Theoretical Study. <i>Sensors</i> , 2016, 16, 658. | 2.1 | 12 |
| 9489 | DNA-Dye-Conjugates: Conformations and Spectra of Fluorescence Probes. <i>PLoS ONE</i> , 2016, 11, e0160229. | 1.1 | 6 |
| 9490 | Computational Investigation of the Interplay of Substrate Positioning and Reactivity in Catechol O-Methyltransferase. <i>PLoS ONE</i> , 2016, 11, e0161868. | 1.1 | 36 |
| 9491 | Conformational Analysis of Molecules: Combined Vibrational Spectroscopy and Density Functional Theory Study. , 2016, , . | | 0 |
| 9492 | Comparative Theoretical Studies on Several Energetic Substituted Dioxin-imidazole Derivatives. <i>Chinese Journal of Chemical Physics</i> , 2016, 29, 349-357. | 0.6 | 1 |
| 9493 | Assessment of Contemporary Theoretical Methods for Bond Dissociation Enthalpies. <i>Chinese Journal of Chemical Physics</i> , 2016, 29, 453-461. | 0.6 | 6 |
| 9494 | Cobalt(II) and copper(II) covalently and non-covalently dichlorido-bridged complexes of an unsymmetrical tripodal pyrazolyl-pyridyl amine ligand: Structures, magnetism and cytotoxicity. <i>Inorganica Chimica Acta</i> , 2016, 451, 102-110. | 1.2 | 23 |
| 9495 | One-Pot Couplingâ€“Couplingâ€“Cyclocondensation Synthesis of Fluorescent Pyrazoles. <i>Journal of Organic Chemistry</i> , 2016, 81, 10328-10338. | 1.7 | 42 |
| 9496 | Comparative density functional theory and density functional tight binding study of arginine and arginine-rich cell penetrating peptide TAT adsorption on anatase TiO ₂ . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 19902-19917. | 1.3 | 24 |
| 9497 | Does DFT+U mimic hybrid density functionals?. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 47 |
| 9498 | The dipolar endofullerene HF@C60. <i>Nature Chemistry</i> , 2016, 8, 953-957. | 6.6 | 167 |
| 9499 | Novel hydrogen- and halogen-bonding anion receptors based on 3-iodopyridinium units. <i>RSC Advances</i> , 2016, 6, 67540-67549. | 1.7 | 29 |
| 9500 | A computational triage approach to the synthesis of novel difluorocyclopentenes and fluorinated cycloheptadienes using thermal rearrangements. <i>Chemical Science</i> , 2016, 7, 6369-6380. | 3.7 | 10 |
| 9501 | Artificial Hydrogenases Based on Cobaloximes and Heme Oxygenase. <i>ChemPlusChem</i> , 2016, 81, 1083-1089. | 1.3 | 25 |
| 9502 | Hydrogenâ€“Bonding Network Anchors the Cyclic Form of Sugar Arylhydrazones. <i>European Journal of Organic Chemistry</i> , 2016, 2016, 3419-3426. | 1.2 | 1 |
| 9503 | Insights on selenium and tellurium diaryldichalcogenides: A benchmark DFT study. <i>Journal of Computational Chemistry</i> , 2016, 37, 1672-1680. | 1.5 | 43 |
| 9504 | Computational study of physisorption and chemisorption of polypyrrole on Hâ€“terminated (111) and (100) nanodiamond facets. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2016, 213, 2672-2679. | 0.8 | 7 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9505 | Doping mechanism of MoO ₃ in 4,4'-Bis(<i>N</i> -carbazolyl)-1,1'-biphenyl: A photoelectron spectroscopic study. <i>Physica Status Solidi (B): Basic Research</i> , 2016, 253, 1697-1706. | 0.7 | 7 |
| 9506 | Synthesis, characterization and activity of imidazolate-bridged and Schiff-base dinuclear complexes as models of Cu,Zn-SOD. A comparative study. <i>Journal of Inorganic Biochemistry</i> , 2016, 163, 162-175. | 1.5 | 21 |
| 9507 | Anion Acceptors Dioxaborinane Contained in Solid State Polymer Electrolyte: Preparation, Characterization, and DFT Calculations. <i>Advanced Functional Materials</i> , 2016, 26, 5930-5939. | 7.8 | 25 |
| 9508 | The substituent effect on the antioxidant capacity of catechols and resorcinols. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 16 |
| 9509 | An Atropisomerically Enforced Phosphoric Acid for Organocatalytic Asymmetric Reactions. <i>European Journal of Organic Chemistry</i> , 2016, 2016, 3208-3216. | 1.2 | 14 |
| 9510 | Modelling materials for solar fuel synthesis by artificial photosynthesis; predicting the optical, electronic and redox properties of photocatalysts. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 074001. | 0.7 | 13 |
| 9511 | <i>Ab initio</i> investigation of 2,2'-bis(4-trifluoromethylphenyl)-5,5'-bibithiazole for the design of efficient organic field-effect transistors. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 339-345. | 1.0 | 12 |
| 9512 | Partitioning the DFT exchange-correlation energy in line with the interacting quantum atoms approach. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 50 |
| 9513 | The 'ceramic approach' in the evaluation of the enantiomeric NorA efflux pump inhibition activity of 2-phenylquinoline derivatives. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2016, 129, 182-189. | 1.4 | 14 |
| 9514 | A series of novel \hat{I}^2 -hydroxyamide based catalysts for borane-mediated enantioselective reductions of prochiral ketones. <i>Tetrahedron: Asymmetry</i> , 2016, 27, 614-622. | 1.8 | 6 |
| 9515 | 2'-prenylated <i>m</i> -dimethoxybenzenes as potent inhibitors of 15-lipoxygenase: inhibitory mechanism and <i>SAR</i> studies. <i>Chemical Biology and Drug Design</i> , 2016, 88, 460-469. | 1.5 | 3 |
| 9516 | Theoretical study of global and local reactivities of coumarin and its hydroxylated derivatives. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 663-669. | 1.0 | 5 |
| 9517 | Theoretical calculation and prediction for experimental design to obtain spin crossover complexes. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1179-1186. | 1.0 | 8 |
| 9518 | Experimental and Theoretical Studies on Corvol Ether Biosynthesis. <i>ChemBioChem</i> , 2016, 17, 146-149. | 1.3 | 19 |
| 9519 | Nickel(II) <i>meso</i> -Hydroxy porphyrin Complexes Revisited: Palladium-Catalysed Synthesis, Electronic Structures of Derived Oxy Radicals, and Oxidative Coupling to a Dioxoporphodimethene Dyad. <i>Chemistry - A European Journal</i> , 2016, 22, 3430-3446. | 1.7 | 26 |
| 9520 | Tungsten Biscorroles: New Chiral Sandwich Compounds. <i>Chemistry - A European Journal</i> , 2016, 22, 6914-6920. | 1.7 | 26 |
| 9521 | Association and Dissociation of Grignard Reagents RMgCl and Their Turbo Variant RMgCl·LiCl. <i>Chemistry - A European Journal</i> , 2016, 22, 7752-7762. | 1.7 | 48 |
| 9522 | Modeling emission features of salicylidene aniline molecular crystals: A QM/QM TM approach. <i>Journal of Computational Chemistry</i> , 2016, 37, 861-870. | 1.5 | 26 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9523 | Scrutinizing "Invisible" astatine: A challenge for modern density functionals. <i>Journal of Computational Chemistry</i> , 2016, 37, 1345-1354. | 1.5 | 42 |
| 9524 | Performance of the OP correlation functional in relation to its formulation: Influence of the exchange component and the effect of incorporating same-spin correlations. <i>Journal of Computational Chemistry</i> , 2016, 37, 1306-1312. | 1.5 | 5 |
| 9525 | Excitation spectra of Bi/Si(001) interfaces. <i>Materialwissenschaft Und Werkstofftechnik</i> , 2016, 47, 120-127. | 0.5 | 4 |
| 9526 | Can We Describe Biological Systems with Quantum Mechanics?. <i>Journal of Physics: Conference Series</i> , 2016, 698, 012009. | 0.3 | 2 |
| 9527 | Synthesis of Five-Porphyrin Nanorings by Using Ferrocene and Corannulene Templates. <i>Angewandte Chemie</i> , 2016, 128, 8498-8502. | 1.6 | 20 |
| 9528 | Importance of Intermolecular Hydrogen Bonding for the Stereochemical Control of Allene-Enone (3+2) Annulations Catalyzed by a Bifunctional, Amino Acid Derived Phosphine Catalyst. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 2022-2027. | 7.2 | 27 |
| 9529 | Improving Memory Performances by Adjusting the Symmetry and Polarity of <i>cis</i> -Fluoroazobenzene-Based Molecules. <i>Chemistry - an Asian Journal</i> , 2016, 11, 512-519. | 1.7 | 9 |
| 9530 | Coordination contributions to protein stability in metal-substituted carbonic anhydrase. <i>Journal of Biological Inorganic Chemistry</i> , 2016, 21, 659-667. | 1.1 | 16 |
| 9531 | Investigation of the Effect of Some Optically Active Imine Compounds on the Enzyme Activities of hCA and hCA under In Vitro Conditions: An Experimental and Theoretical Study. <i>Journal of Biochemical and Molecular Toxicology</i> , 2016, 30, 277-286. | 1.4 | 1 |
| 9532 | Tuning the push-pull configuration for efficient second-order nonlinear optical properties in some chalcone derivatives. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 68, 95-105. | 1.3 | 77 |
| 9533 | Theoretical Analysis on the Importance of Achiral Unidentate Ligands to Electronic Circular Dichroism of <i>cis</i> -Bis(ethylenediamine) Cobalt(III) Complexes. <i>Inorganic Chemistry</i> , 2016, 55, 6949-6960. | 1.9 | 4 |
| 9534 | Core electron excitations in U^{4+} : modelling of the $nd^{10}5f^{2}n^{\prime}$ $nd^{9}5f^{3}$ transitions with $n = 3, 4$ and 5 by ligand field tools and density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 19020-19031. | 1.3 | 21 |
| 9535 | Twisted olefinic building blocks for low bandgap polymers in solar cells and ambipolar field-effect transistors. <i>Journal of Polymer Science Part A</i> , 2016, 54, 889-899. | 2.5 | 7 |
| 9536 | On the possibility of phase transitions with the formation of SiO ₂ peroxide forms in the earth mantle and their effect on mantle convection. <i>Journal of Structural Chemistry</i> , 2016, 57, 417-421. | 0.3 | 3 |
| 9537 | Pairing of carbon atoms in low-energy deltahedral dicarbogallane structures derived from vertex expansion of closo deltahedra. <i>Journal of Organometallic Chemistry</i> , 2016, 819, 173-181. | 0.8 | 3 |
| 9538 | Atmospheric chemistry of CF ₃ (CX ₂) ₂ CH ₂ OH: rate coefficients and temperature dependence of reactions with chlorine atoms and the subsequent pathways of alkyl and alkoxy radicals (X = H, F). <i>RSC Advances</i> , 2016, 6, 63954-63964. | 1.7 | 10 |
| 9539 | Copper(II) and Zinc(II) Complexes of Conformationally Constrained Polyazamacrocycles as Efficient Catalysts for RNA Model Substrate Cleavage in Aqueous Solution at Physiological pH. <i>Chemistry - A European Journal</i> , 2016, 22, 10426-10437. | 1.7 | 20 |
| 9540 | Baeckeins J and K, Two Novel <i>cis</i> -Methylated Biflavonoids from the Roots of <i>Baeckea frutescens</i> and Their Cytoprotective Activities. <i>Helvetica Chimica Acta</i> , 2016, 99, 499-505. | 1.0 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9541 | Topological analysis of the electron delocalization range. Journal of Computational Chemistry, 2016, 37, 1993-2005. | 1.5 | 9 |
| 9542 | Boron Difluoride Curcuminoid Fluorophores with Enhanced Two-Photon Excited Fluorescence Emission and Versatile Living-Cell Imaging Properties. Chemistry - A European Journal, 2016, 22, 5219-5232. | 1.7 | 77 |
| 9543 | Comparative Computational Study of Hydrogen Abstraction Reactions of $CY_3H + XO^{\bullet}$ (X, Y = F, Cl, and Tj ETQq0.0 0 rgBT ₁ /Overlock | 0.4 | 1 |
| 9544 | Geometric and electronic structures of silicon fluorides ($N = 4$) and potential energy surfaces for dissociation reactions $SiF_4 + F^{\bullet}$ and $SiF_4 + F_2^{\bullet}$. International Journal of Quantum Chemistry, 2016, 116, 1358-1361. | 1 | 1 |
| 9545 | NMR absolute shielding scale and nuclear magnetic dipole moment of ^{207}Pb . Physical Chemistry Chemical Physics, 2016, 18, 16483-16490. | 1.3 | 23 |
| 9546 | Mild $C^{\bullet}H/C^{\bullet}C$ Activation by Zr -Selective Cobalt Catalysis. Angewandte Chemie - International Edition, 2016, 55, 7408-7412. | 7.2 | 166 |
| 9547 | Kinetic and Theoretical Investigation of Iron(III)-Catalyzed Silane Chlorination. ChemCatChem, 2016, 8, 584-592. | 1.8 | 3 |
| 9548 | Interplay of Exciton Coupling and Large-Amplitude Motions in the Vibrational Circular Dichroism Spectrum of Dehydroquinidine. Chemistry - A European Journal, 2016, 22, 704-715. | 1.7 | 20 |
| 9549 | Macrocyclic-Based Hydroxamate Ligands for Complexation and Immunoconjugation of ^{89}Zr for Positron Emission Tomography (PET) Imaging. ChemPlusChem, 2016, 81, 274-281. | 1.3 | 55 |
| 9550 | Importance of Intermolecular Hydrogen Bonding for the Stereochemical Control of Allene-Enone (3+2) Annulations Catalyzed by a Bifunctional, Amino Acid Derived Phosphine Catalyst. Angewandte Chemie, 2016, 128, 2062-2067. | 1.6 | 7 |
| 9551 | Hochaktive Titanocen-Katalysatoren für Epoxid-Hydrosilylierungen – Synthese, Theorie, Kinetik, EPR-Spektroskopie. Angewandte Chemie, 2016, 128, 7801-7805. | 1.6 | 27 |
| 9552 | Mild $C^{\bullet}H/C^{\bullet}C$ Activation by Zr -Selective Cobalt Catalysis. Angewandte Chemie, 2016, 128, 7534-7538. | 1.6 | 52 |
| 9553 | O -hydroxy Schiff Bases Derived from 2-Hydroxy-4-methoxy Benzaldehyde: Synthesis, X-Ray Studies and Hydrogen Bonding Attributes. Molecular Crystals and Liquid Crystals, 2016, 629, 146-157. | 0.4 | 8 |
| 9554 | Electronic Properties of Cyclacenes from TAO-DFT. Scientific Reports, 2016, 6, 37249. | 1.6 | 50 |
| 9555 | Celebrating Our 120th Anniversary. Journal of Physical Chemistry B, 2016, 120, 12417-12419. | 1.2 | 1 |
| 9556 | Celebrating Our 120th Anniversary. Journal of Physical Chemistry Letters, 2016, 7, 4977-4979. | 2.1 | 0 |
| 9557 | Effect of conformation on UV-Vis absorption spectra of disazo reactive red dyes. Wuhan University Journal of Natural Sciences, 2016, 21, 512-518. | 0.2 | 2 |
| 9558 | Quantifying electron transfer reactions in biological systems: what interactions play the major role?. Scientific Reports, 2016, 5, 18446. | 1.6 | 67 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9559 | Insights into the geometries, electronic and magnetic properties of neutral and charged palladium clusters. <i>Scientific Reports</i> , 2016, 6, 19656. | 1.6 | 73 |
| 9560 | Redox Active Ion-Paired Excited States Undergo Dynamic Electron Transfer. <i>Journal of the American Chemical Society</i> , 2016, 138, 16815-16826. | 6.6 | 38 |
| 9561 | Diffusion Monte Carlo Study of the Parallel Displaced Form of the Benzene Dimer. <i>ACS Symposium Series</i> , 2016, , 107-117. | 0.5 | 3 |
| 9562 | Extraction of Water and Speciation of Trivalent Lanthanides and Americium in Organophosphorus Extractants. <i>Inorganic Chemistry</i> , 2016, 55, 12675-12685. | 1.9 | 18 |
| 9563 | Osmium(II) Complexes Containing a Dianionic CCCC-Donor Tetradentate Ligand. <i>Organometallics</i> , 2016, 35, 3981-3995. | 1.1 | 31 |
| 9564 | The Reductive Cleavage Mechanism and Complex Stability of Glutathionyl-Cobalamin in Acidic Media. <i>Electroanalysis</i> , 2016, 28, 2743-2753. | 1.5 | 4 |
| 9565 | Energetics of Radical Formation in Eumelanin Building Blocks: Implications for Understanding Photoprotection Mechanisms in Eumelanin. <i>Journal of Physical Chemistry A</i> , 2016, 120, 10018-10022. | 1.1 | 0 |
| 9566 | Assessing covalency in equatorial U-N bonds: density based measures of bonding in BTP and isoamethyrin complexes of uranyl. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 16830-16839. | 1.3 | 24 |
| 9567 | Predictive coupled-cluster isomer orderings for some Si _n C _m (<i>m</i> , <i>n</i> ≤ 12) clusters: A pragmatic comparison between DFT and complete basis limit coupled-cluster benchmarks. <i>Journal of Chemical Physics</i> , 2016, 145, 024312. | 1.2 | 14 |
| 9568 | Reactivity of alkynylsilanes towards B-halogeno-1,3,2-diselenaborolanes with an annelated dicarba-closo-dodecaborane(12) unit. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2016, 71, 979-992. | 0.3 | 1 |
| 9569 | Combinatorial Broadening Mechanism of O-H Stretching Bands in H-Bonded Molecular Clusters. <i>Journal of Applied Spectroscopy</i> , 2016, 83, 350-357. | 0.3 | 4 |
| 9570 | Matrix effects in the C 1s photoabsorption spectra of condensed naphthalene. <i>Journal of Chemical Physics</i> , 2016, 145, 234307. | 1.2 | 4 |
| 9571 | Stereo sensitivity of exchange interactions in NiII and CuII heterospin complexes with 5-formylpyrrolyl-substituted nitroxides. <i>Russian Chemical Bulletin</i> , 2016, 65, 666-674. | 0.4 | 9 |
| 9572 | SCAN-based hybrid and double-hybrid density functionals from models without fitted parameters. <i>Journal of Chemical Physics</i> , 2016, 144, 044114. | 1.2 | 126 |
| 9573 | Tuning the charge states of CrW2O9 clusters deposited on perfect and defective MgO(001) surfaces with different color centers: A comprehensive DFT study. <i>Journal of Chemical Physics</i> , 2016, 144, 174706. | 1.2 | 4 |
| 9574 | Molecular dynamics simulation elucidates the preferential binding affinity of sodium and tetramethylammonium ions for tetrameric Nafion unit under aqueous conditions. <i>RSC Advances</i> , 2016, 6, 97961-97968. | 1.7 | 6 |
| 9575 | Path optimization by a variational reaction coordinate method. II. Improved computational efficiency through internal coordinates and surface interpolation. <i>Journal of Chemical Physics</i> , 2016, 144, 184101. | 1.2 | 5 |
| 9576 | Multicomponent density functional theory embedding formulation. <i>Journal of Chemical Physics</i> , 2016, 145, 044106. | 1.2 | 20 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9577 | Conformational differences and intermolecular C-H...N interactions in three polymorphs of a bis(pyridinyl)-substituted benzimidazole. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2016, 72, 867-874. | 0.2 | 6 |
| 9578 | Theoretical study on electronic structures, spectra, and charge transporting properties of two Pt(II) complexes with triazenido ligands. <i>Russian Journal of General Chemistry</i> , 2016, 86, 2817-2826. | 0.3 | 1 |
| 9579 | Polarization-sensitive electro-optic detection of terahertz wave using three different types of crystal symmetry: Toward broadband polarization spectroscopy. <i>Applied Physics Letters</i> , 2016, 108, . | 1.5 | 14 |
| 9580 | Hydrogenation and dehydrogenation of interstellar PAHs: Spectral characteristics and H ₂ formation. <i>Astronomy and Astrophysics</i> , 2016, 595, A23. | 2.1 | 61 |
| 9581 | A cumulant functional for static and dynamic correlation. <i>Journal of Chemical Physics</i> , 2016, 145, 084106. | 1.2 | 9 |
| 9582 | Signatures of Size-Dependent Structural Patterns in Hydrated Copper(I) Clusters, Cu ⁺ (H ₂ O) _n . <i>Journal of Physical Chemistry A</i> , 2016, 120, 10252-10263. | 1.1 | 7 |
| 9583 | Stable isomers and electronic, vibrational, and optical properties of WS ₂ nano-clusters: A first-principles study. <i>Journal of Chemical Physics</i> , 2016, 145, 214303. | 1.2 | 6 |
| 9584 | The QTP family of consistent functionals and potentials in Kohn-Sham density functional theory. <i>Journal of Chemical Physics</i> , 2016, 145, 034107. | 1.2 | 68 |
| 9585 | Can dispersion corrections annihilate the dispersion-driven nano-aggregation of non-polar groups? An <i>ab initio</i> molecular dynamics study of ionic liquid systems. <i>Journal of Chemical Physics</i> , 2016, 145, 204502. | 1.2 | 13 |
| 9586 | The discovery of the hydrogen bond from p-Nitrothiophenol by Raman spectroscopy: Guideline for the thioalcohol molecule recognition tool. <i>Scientific Reports</i> , 2016, 6, 31981. | 1.6 | 26 |
| 9587 | Left-right correlation in coupled F-center defects. <i>Journal of Chemical Physics</i> , 2016, 145, 054703. | 1.2 | 5 |
| 9588 | Induction and Rationalization of Supramolecular Chirality in the Tweezer-Diamine Complexes: Insights from Experimental and DFT Studies. <i>Inorganic Chemistry</i> , 2016, 55, 13014-13026. | 1.9 | 19 |
| 9589 | Calibrating Reaction Enthalpies: Use of Density Functional Theory and the Correlation Consistent Composite Approach in the Design of Photochromic Materials. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9982-9997. | 1.1 | 6 |
| 9590 | Extension of the Slipids Force Field to Polyunsaturated Lipids. <i>Journal of Physical Chemistry B</i> , 2016, 120, 12826-12842. | 1.2 | 39 |
| 9591 | Quantum Monte Carlo Calculations on the Anomeric Effect. <i>ACS Symposium Series</i> , 2016, , 89-105. | 0.5 | 1 |
| 9592 | Tuning dissociation using isoelectronically doped graphene and hexagonal boron nitride: Water and other small molecules. <i>Journal of Chemical Physics</i> , 2016, 144, 154706. | 1.2 | 20 |
| 9593 | Rungs 1 to 4 of DFT Jacobian's ladder: Extensive test on the lattice constant, bulk modulus, and cohesive energy of solids. <i>Journal of Chemical Physics</i> , 2016, 144, 204120. | 1.2 | 191 |
| 9594 | Blind test of density-functional-based methods on intermolecular interaction energies. <i>Journal of Chemical Physics</i> , 2016, 145, 124105. | 1.2 | 97 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9595 | Time-Dependent Density Functional Theoretical Investigation of Photoinduced Excited-State Intramolecular Dual Proton Transfer in Diformyl Dipyrromethanes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9894-9906. | 1.1 | 10 |
| 9596 | Excess electrons in methanol clusters: Beyond the one-electron picture. <i>Journal of Chemical Physics</i> , 2016, 145, 164313. | 1.2 | 5 |
| 9597 | A polarizable QM/MM approach to the molecular dynamics of amide groups solvated in water. <i>Journal of Chemical Physics</i> , 2016, 144, 114504. | 1.2 | 14 |
| 9598 | Celebrating Our 120th Anniversary. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9679-9681. | 1.1 | 3 |
| 9599 | Celebrating Our 120th Anniversary. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27731-27733. | 1.5 | 0 |
| 9600 | Relationship between cap structure and energy gap in capped carbon nanotubes. <i>Journal of Chemical Physics</i> , 2016, 145, 024702. | 1.2 | 0 |
| 9601 | Perspective: Kohn-Sham density functional theory descending a staircase. <i>Journal of Chemical Physics</i> , 2016, 145, 130901. | 1.2 | 243 |
| 9602 | Short- and long-range corrected hybrid density functionals with the D3 dispersion corrections. <i>Journal of Chemical Physics</i> , 2016, 145, 204101. | 1.2 | 26 |
| 9603 | Assessment of a composite CC2/DFT procedure for calculating $\sigma^* \leftarrow 0$ excitation energies of organic molecules. <i>Molecular Physics</i> , 2016, 114, 3448-3463. | 0.8 | 20 |
| 9604 | The Heaviest Possible Ternary Trihalogen Species, $\text{IAtBr}^{\text{+}}$, Evidenced in Aqueous Solution: An Experimental Performance Driven by Computations. <i>Angewandte Chemie</i> , 2016, 128, 15595-15598. | 1.6 | 8 |
| 9605 | Transition from Molecular Vibrations to Phonons in Atomically Precise Cadmium Selenide Quantum Dots. <i>Journal of the American Chemical Society</i> , 2016, 138, 16754-16763. | 6.6 | 36 |
| 9606 | Hydrogen migration in hypoelectronic bicapped metallocene structures. <i>RSC Advances</i> , 2016, 6, 87096-87102. | 1.7 | 0 |
| 9607 | The impact of electron correlations on the energetics and stability of silicon nanoclusters. <i>Journal of Chemical Physics</i> , 2016, 145, 074313. | 1.2 | 7 |
| 9608 | Synthesis and structure of 3-[[ary] (hetaryl)amino]methylene]chromane-2,4-diones and their metal complexes. <i>Russian Journal of General Chemistry</i> , 2016, 86, 2492-2500. | 0.3 | 1 |
| 9609 | Perspective: How good is DFT for water?. <i>Journal of Chemical Physics</i> , 2016, 144, 130901. | 1.2 | 571 |
| 9610 | Efficient Hydrosilylation of Acetophenone with a New Anthraquinonic Amide-Based Iron Precatalyst. <i>Organometallics</i> , 2016, 35, 4083-4089. | 1.1 | 20 |
| 9611 | Gold(I) Complexes $[\text{N}(\text{C}_3\text{F}_7)\text{C}(\text{Dipp})\text{N}]_2\text{AuL}$ (L = Ethylene, tert-butyl Isocyanide, etc.) and Their Catalytic Modes. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 5435-5444. | 1.0 | 1 |
| 9612 | A polarizable continuum model for molecules at spherical diffuse interfaces. <i>Journal of Chemical Physics</i> , 2016, 144, 124103. | 1.2 | 13 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9613 | The effect of basis set and exchange-correlation functional on time-dependent density functional theory calculations within the Tamm-Dancoff approximation of the x-ray emission spectroscopy of transition metal complexes. Journal of Chemical Physics, 2016, 144, 114104. | 1.2 | 26 |
| 9614 | Theoretical and experimental study of mononuclear Cu(II) acetate-bipyridine complex. Journal of Structural Chemistry, 2016, 57, 1348-1354. | 0.3 | 4 |
| 9615 | Vertical excitation energies from the adiabatic connection. Journal of Chemical Physics, 2016, 145, 194107. | 1.2 | 24 |
| 9616 | Simulation of UV/Vis Spectra of CyMe4BTBP and Some of its Degradation Products. Procedia Chemistry, 2016, 21, 509-516. | 0.7 | 1 |
| 9617 | Enhanced ordering reduces electric susceptibility of liquids confined to graphene slit pores. Scientific Reports, 2016, 6, 27406. | 1.6 | 13 |
| 9618 | Targeting excited states in all-trans polyenes with electron-pair states. Journal of Chemical Physics, 2016, 145, 234105. | 1.2 | 35 |
| 9619 | Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. Journal of Chemical Physics, 2016, 145, 234306. | 1.2 | 25 |
| 9620 | A hydrated ion model of [UO ₂] ²⁺ in water: Structure, dynamics, and spectroscopy from classical molecular dynamics. Journal of Chemical Physics, 2016, 145, 224502. | 1.2 | 17 |
| 9621 | Supramolecular polymerization of a prebiotic nucleoside provides insights into the creation of sequence-controlled polymers. Scientific Reports, 2016, 6, 18891. | 1.6 | 5 |
| 9622 | Charged vanadium-benzene multidecker clusters: DFT and quantum Monte Carlo study. Journal of Chemical Physics, 2016, 144, 064303. | 1.2 | 4 |
| 9623 | Estimation of steric hindrances at the dimerization of free organic radicals. Russian Journal of Organic Chemistry, 2016, 52, 1576-1586. | 0.3 | 5 |
| 9624 | Push it to the limit: Characterizing the convergence of common sequences of basis sets for intermolecular interactions as described by density functional theory. Journal of Chemical Physics, 2016, 144, 194306. | 1.2 | 41 |
| 9625 | A DFT investigation on the structural and antioxidant properties of new isolated interglycosidic O-(1- β -D-galactopyranosyl) Tj ETQq0 0,0 rgBT /Overlock 10 | 0.8 | 51 |
| 9626 | Exciton Splitting of Adsorbed and Free 4-Nitroazobenzene Dimers: A Quantum Chemical Study. Journal of Physical Chemistry A, 2016, 120, 3055-3070. | 1.1 | 16 |
| 9627 | Exploring the Photodeactivation Pathways of Pt[O ^N C ^N] Complexes: A Theoretical Perspective. ChemPhysChem, 2016, 17, 69-77. | 1.0 | 18 |
| 9628 | 211 At-labeled agents for alpha-immunotherapy: On the <i>in vivo</i> stability of astatine-agent bonds. European Journal of Medicinal Chemistry, 2016, 116, 156-164. | 2.6 | 28 |
| 9629 | A complete synergy on the experimental and theoretical study of the pyridine derivatives " 2-Hydroxy-5-Nitropyridine and 2-Chloro-5-Nitropyridine. Journal of Molecular Structure, 2016, 1117, 121-134. | 1.8 | 9 |
| 9630 | Relativistic coupled-cluster calculations of the ¹⁷³ Yb nuclear quadrupole coupling constant for the YbF molecule. Molecular Physics, 2016, 114, 1110-1117. | 0.8 | 10 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9631 | Generalized relativistic effective core potentials for actinides. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 301-315. | 1.0 | 47 |
| 9632 | A dataset of highly accurate homolytic Ni-Br bond dissociation energies obtained by Means of W2 theory. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 52-60. | 1.0 | 28 |
| 9633 | Reaction mechanism and regioselectivity for chelated Ru-catalyzed AROCM of endic anhydride and propene: A DFT study. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 35-41. | 1.0 | 2 |
| 9634 | Hybrid Density Functionals Applied to Complex Solid Catalysts: Successes, Limitations, and Prospects. <i>Catalysis Letters</i> , 2016, 146, 861-885. | 1.4 | 31 |
| 9635 | Conformations, equilibrium thermodynamics and rotational barriers of secondary thiobenzanilides. <i>Tetrahedron</i> , 2016, 72, 2072-2083. | 1.0 | 7 |
| 9636 | Local electric fields and molecular properties in heterogeneous environments through polarizable embedding. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 10070-10080. | 1.3 | 60 |
| 9637 | Insights into the Thiamine Diphosphate Enzyme Activation Mechanism: Computational Model for Transketolase Using a Quantum Mechanical/Molecular Mechanical Method. <i>Biochemistry</i> , 2016, 55, 2144-2152. | 1.2 | 12 |
| 9638 | Luminescent osmium(ii) bi-1,2,3-triazol-4-yl complexes: photophysical characterisation and application in light-emitting electrochemical cells. <i>Dalton Transactions</i> , 2016, 45, 7748-7757. | 1.6 | 45 |
| 9639 | Kinetics and thermochemistry of hydrolysis mechanism of a novel anticancer agent trans-[PtCl ₂ (dimethylamine)(isopropylamine)]: A DFT study. <i>Chemical Physics Letters</i> , 2016, 651, 216-220. | 1.2 | 1 |
| 9640 | Rhodocomatulin-Type Anthraquinones from the Australian Marine Invertebrates <i>Clathria hirsuta</i> and <i>Comatula rotalaria</i> . <i>Journal of Natural Products</i> , 2016, 79, 946-953. | 1.5 | 16 |
| 9641 | A Series of Novel Derivatives with Giant Second Hyperpolarizabilities, Based on Radiannulenes, Tetrathiafulvalene, Nickel Dithiolene, and Their Lithiated Analogues. <i>Journal of Physical Chemistry C</i> , 2016, 120, 9419-9435. | 1.5 | 25 |
| 9642 | Impact of Ligand and Silane on the Regioselectivity in Catalytic Aldehyde-Alkyne Reductive Couplings: A Theoretical Study. <i>Organometallics</i> , 2016, 35, 1114-1124. | 1.1 | 23 |
| 9643 | New approaches for the calibration of exchange-energy densities in local hybrid functionals. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21133-21144. | 1.3 | 43 |
| 9644 | Synthesis of a mononuclear, non-square-planar chromium(ii) bis(alkoxide) complex and its reactivity toward organic carbonyls and CO ₂ . <i>Dalton Transactions</i> , 2016, 45, 9794-9804. | 1.6 | 22 |
| 9645 | A theoretical design and investigation on Zn-porphyrin-polyoxometalate hybrids with different IR-linkers for searching high performance sensitizers of p-type dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2016, 130, 168-175. | 2.0 | 27 |
| 9646 | Exploring photochemistry of p-bromophenylsulfonyl, p-tolylsulfonyl and methylsulfonyl azides by ultrafast UV-pump-IR-probe spectroscopy and computations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8662-8672. | 1.3 | 17 |
| 9647 | Isomerization and fragmentation pathways of 1,2-azaborine. <i>Journal of Computational Chemistry</i> , 2016, 37, 110-116. | 1.5 | 8 |
| 9648 | Alkene Epoxidation Catalyzed by Ti-Containing Polyoxometalates: Unprecedented ¹² Oxygen Transfer Mechanism. <i>Inorganic Chemistry</i> , 2016, 55, 6080-6084. | 1.9 | 40 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9649 | Comparison of Three Efficient Approximate Exact-Exchange Algorithms: The Chain-of-Spheres Algorithm, Pair-Atomic Resolution-of-the-Identity Method, and Auxiliary Density Matrix Method. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3514-3522. | 2.3 | 29 |
| 9650 | Theoretical investigation of 2-(iminomethyl)phenol in the gas phase as a prototype of ultrafast excited-state intramolecular proton transfer. <i>Chemical Physics Letters</i> , 2016, 657, 113-118. | 1.2 | 12 |
| 9651 | Electronic and Optical Properties of the Narrowest Armchair Graphene Nanoribbons Studied by Density Functional Methods. <i>Australian Journal of Chemistry</i> , 2016, 69, 960. | 0.5 | 10 |
| 9652 | Hydrogen bonding at C=Se acceptors in selenoureas, selenoamides and selones. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 317-325. | 0.5 | 23 |
| 9653 | Computational and ³¹ P NMR studies of moisture-metastable cyclic diaminophosphine oxide preligands. <i>Polyhedron</i> , 2016, 105, 123-136. | 1.0 | 3 |
| 9654 | Complex Orbitals, Multiple Local Minima, and Symmetry Breaking in Perdew's Zunger Self-Interaction Corrected Density Functional Theory Calculations. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3195-3207. | 2.3 | 54 |
| 9655 | Novel Dimeric <i>o</i> -Carboranyl Triarylborane: Intriguing Ratiometric Color-Tunable Sensor via Aggregation-Induced Emission by Fluoride Anions. <i>Organometallics</i> , 2016, 35, 1771-1777. | 1.1 | 68 |
| 9656 | Controlling electron emission from the photoactive yellow protein chromophore by substitution at the coumaric acid group. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 10329-10336. | 1.3 | 18 |
| 9657 | Three new Ag(I) thiosaccharinate complexes: Synthesis, structural studies, spectral characterization and theoretical analysis. <i>Inorganica Chimica Acta</i> , 2016, 450, 39-49. | 1.2 | 11 |
| 9658 | Density Functional Theory. <i>Graduate Texts in Physics</i> , 2016, , 99-110. | 0.1 | 1 |
| 9659 | Anisotropic Effects of Oxygen Vacancies on Electrochromic Properties and Conductivity of β -Monoclinic WO_3 . <i>Journal of Physical Chemistry C</i> , 2016, 120, 11716-11726. | 1.5 | 70 |
| 9660 | Molecular dynamics based cohesive zone modeling of Al (metal)-Cu ₅₀ Zr ₅₀ (metallic glass) interfacial mechanical behavior and investigation of dissipative mechanisms. <i>Materials and Design</i> , 2016, 105, 41-50. | 3.3 | 55 |
| 9661 | Stereoselective synthesis and application of tridentate aminodiols derived from (+)-pulegone. <i>Tetrahedron: Asymmetry</i> , 2016, 27, 480-486. | 1.8 | 14 |
| 9662 | Chlorine Para-Substitution of 1-Phenylethanol: Resonant Photoionization Spectroscopy and Quantum Chemical Calculations of Hydrated and Diastereomeric Complexes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5023-5031. | 1.1 | 1 |
| 9663 | Benchmark Calculations for Bond Dissociation Enthalpies of Unsaturated Methyl Esters and the Bond Dissociation Enthalpies of Methyl Linolenate. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4025-4036. | 1.1 | 49 |
| 9664 | Photoelectron Velocity Map Imaging Spectroscopy of Lead Tetracarbonyl-Iron Anion $\text{PbFe}(\text{CO})_4^+$. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3533-3538. | 1.1 | 15 |
| 9665 | Closing the Gap: Preparation and Characterization of the First Half-Open and Open Manganocene Complexes. <i>Organometallics</i> , 2016, 35, 1986-1994. | 1.1 | 9 |
| 9666 | Synthesis and piezochromic luminescence study of a coumarin hydrozone compound. <i>Chemical Communications</i> , 2016, 52, 7387-7389. | 2.2 | 26 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9667 | Iodide-bridged dinuclear copper(I) complex with cyanopyrazine and its conversion into bis(tetrazolato)copper(II) complex via [3+2] cycloaddition: synthesis, structure and self-assembly. <i>Journal of the Iranian Chemical Society</i> , 2016, 13, 1713-1721. | 1.2 | 3 |
| 9668 | Probing the Reactivity of the Ce•O Multiple Bond in a Cerium(IV) Oxo Complex. <i>Inorganic Chemistry</i> , 2016, 55, 10003-10012. | 1.9 | 30 |
| 9669 | Revised Damping Parameters for the D3 Dispersion Correction to Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2197-2203. | 2.1 | 305 |
| 9670 | Catecholase activity of Mannich-based dinuclear Cu ^{II} complexes with theoretical modeling: new insight into the solvent role in the catalytic cycle. <i>New Journal of Chemistry</i> , 2016, 40, 6623-6635. | 1.4 | 29 |
| 9671 | Dipicolylamine coupled rhodamine dyes: new clefts for highly selective naked eye sensing of Cu ²⁺ and CN ⁻ ions. <i>RSC Advances</i> , 2016, 6, 47802-47812. | 1.7 | 17 |
| 9672 | Theoretical Study of Quantum Conductance of Conjugated and Nonconjugated Molecular Wire Junctions. <i>Journal of Physical Chemistry C</i> , 2016, 120, 11820-11830. | 1.5 | 16 |
| 9673 | Graphene quantum dots: structural integrity and oxygen functional groups for high sulfur/sulfide utilization in lithium sulfur batteries. <i>NPG Asia Materials</i> , 2016, 8, e272-e272. | 3.8 | 105 |
| 9674 | Insights into Bulk Electrolyte Effects on the Operative Voltage of Electrochemical Double-Layer Capacitors. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12325-12336. | 1.5 | 15 |
| 9675 | Adsorbate-Induced Changes in Magnetic Interactions in Fe ₂ (dobdc) with Adsorbed Hydrocarbon Molecules. <i>Journal of Physical Chemistry C</i> , 2016, 120, 9933-9948. | 1.5 | 15 |
| 9676 | Diindeno-fusion of an anthracene as a design strategy for stable organic biradicals. <i>Nature Chemistry</i> , 2016, 8, 753-759. | 6.6 | 302 |
| 9677 | Phase transition, thermal dissociation and dynamics of NH ₃ ligands in [Cd(NH ₃) ₄](ReO ₄) ₂ . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 164, 24-32. | 2.0 | 7 |
| 9678 | Phase transition and NH ₃ dynamics in [Ni(NH ₃) ₄](ReO ₄) ₂ studied by infrared absorption, X-ray powder diffraction and neutron scattering methods. <i>Chemical Physics</i> , 2016, 469-470, 9-15. | 0.9 | 2 |
| 9679 | Photoelectron spectra and electronic structure of nitrogen analogues of boron β^2 -diketonates. <i>Journal of Molecular Structure</i> , 2016, 1115, 1-7. | 1.8 | 4 |
| 9680 | Averaged Solvent Embedding Potential Parameters for Multiscale Modeling of Molecular Properties. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1684-1695. | 2.3 | 42 |
| 9681 | Enhanced Photoluminescence Quantum Yields through Excimer Formation of Cyclometalated Platinum(II) N-Heterocyclic Carbene Complexes. <i>Organometallics</i> , 2016, 35, 673-680. | 1.1 | 62 |
| 9682 | Novel aluminum-BODIPY dyads: intriguing dual-emission via photoinduced energy transfer. <i>Dalton Transactions</i> , 2016, 45, 5825-5832. | 1.6 | 15 |
| 9683 | Captodative substitution induced acceleration effect towards 4 π electrocyclic ring-opening of substituted cyclobutenes. <i>RSC Advances</i> , 2016, 6, 25503-25510. | 1.7 | 6 |
| 9684 | Another step toward DNA selective targeting: Ni ^{II} and Cu ^{II} complexes of a Schiff base ligand able to bind gene promoter G-quadruplexes. <i>Dalton Transactions</i> , 2016, 45, 7758-7767. | 1.6 | 49 |

| # | ARTICLE | IF | CITATIONS |
|------|---|------|-----------|
| 9685 | Advances on the Determination of the Astatine Pourbaix Diagram: Predominance of $\text{AtO}(\text{OH})_2^{\text{+}}$ over $\text{At}^{\text{+}}$ in Basic Conditions. <i>Chemistry - A European Journal</i> , 2016, 22, 2964-2971. | 1.7 | 46 |
| 9686 | HFEPR and Computational Studies on the Electronic Structure of a High-Spin Oxidiron(IV) Complex in Solution. <i>Inorganic Chemistry</i> , 2016, 55, 3933-3945. | 1.9 | 11 |
| 9687 | A quantum chemical study of the molecular structure of zinc(II) and boron(II) complexes with monoiodo and dibromo substituted dipyrines. <i>Journal of Structural Chemistry</i> , 2016, 57, 25-32. | 0.3 | 17 |
| 9688 | Enantioselective Oxidative Rearrangements with Chiral Hypervalent Iodine Reagents. <i>Chemistry - A European Journal</i> , 2016, 22, 4030-4035. | 1.7 | 78 |
| 9689 | Optical properties of the dibenzothiazolylphenol molecular crystals through ONIOM calculations: the effect of the electrostatic embedding scheme. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 14 |
| 9690 | The mechanisms for N-heterocyclic olefin-catalyzed formation of cyclic carbonate from CO_2 and propargylic alcohols. <i>Journal of Molecular Modeling</i> , 2016, 22, 94. | 0.8 | 11 |
| 9691 | 4-Component relativistic calculations of L_{3^+} ionization and excitations for the isoelectronic species UO_2^{2+} , OUN^+ and UN_2 . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21010-21023. | 1.3 | 24 |
| 9692 | Chlorodiphenyltin(IV) dithiocarbamate complexes as chemodosimeters and host for anions and neutral compounds in solution. <i>Polyhedron</i> , 2016, 111, 132-142. | 1.0 | 9 |
| 9693 | Quantum Mechanics/Molecular Mechanics Modeling of Drug Metabolism: Mexiletine N-Hydroxylation by Cytochrome P450 1A2. <i>Chemical Research in Toxicology</i> , 2016, 29, 963-971. | 1.7 | 27 |
| 9694 | Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. <i>Chemical Reviews</i> , 2016, 116, 5301-5337. | 23.0 | 312 |
| 9695 | Trends in the Spin States and Mean Static Dipole Polarizability of the Group VIIIA Metallocenes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2771-2778. | 1.1 | 14 |
| 9696 | An air-stable $\text{Dy}(\text{III})$ single-ion magnet with high anisotropy barrier and blocking temperature. <i>Chemical Science</i> , 2016, 7, 5181-5191. | 3.7 | 477 |
| 9697 | Molecular modelling of translocation of biomolecules in carbon nanotubes: method, mechanism and application. <i>Molecular Simulation</i> , 2016, 42, 827-835. | 0.9 | 17 |
| 9698 | Possible reasons that catalytic reactivity towards low-temperature CO oxidation has not been found in Au_3^+ cluster. <i>Computational and Theoretical Chemistry</i> , 2016, 1085, 75-81. | 1.1 | 6 |
| 9699 | A PW91-like exchange with a simple analytical form. <i>Chemical Physics Letters</i> , 2016, 651, 268-273. | 1.2 | 16 |
| 9700 | Synthesis of Functionalized 1,3,2-Benzodiazaborole Cores Using Bench-Stable Components. <i>Journal of Organic Chemistry</i> , 2016, 81, 3771-3779. | 1.7 | 21 |
| 9701 | Expanding the (cross-)hyperconjugation of 1,4-disilacyclohexa-2,5-dienes to larger monomers and oligomers: a computational investigation. <i>RSC Advances</i> , 2016, 6, 36961-36970. | 1.7 | 8 |
| 9702 | Dispersion-Corrected Mean-Field Electronic Structure Methods. <i>Chemical Reviews</i> , 2016, 116, 5105-5154. | 23.0 | 1,032 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9703 | Expensive tripodal rotation in η^6 -chromium tricarbonyl complexes of phosphabenzene-Insights from DFT study. <i>Computational and Theoretical Chemistry</i> , 2016, 1084, 103-108. | 1.1 | 2 |
| 9704 | Solvent effects on lasing characteristics for Rh B laser dye. <i>Journal of Luminescence</i> , 2016, 169, 227-232. | 1.5 | 5 |
| 9705 | Study on the removal of benzisothiazolinone biocide and its toxicity: The effectiveness of ozonation. <i>Chemical Engineering Journal</i> , 2016, 300, 376-383. | 6.6 | 44 |
| 9706 | Parquet compounds on the basis of eight- and twelve-membered structure blocks: Quantum-chemical study. <i>Russian Journal of Organic Chemistry</i> , 2016, 52, 268-282. | 0.3 | 3 |
| 9707 | Global hybrid exchange energy functional with correct asymptotic behavior of the corresponding potential. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 7 |
| 9708 | Tautomerization mechanism and spectral properties of porphyrin-glucose complexes as models of antibacterial material. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 10 |
| 9709 | Solution Structures of Highly Active Molecular Ir Water-Oxidation Catalysts from Density Functional Theory Combined with High-Energy X-ray Scattering and EXAFS Spectroscopy. <i>Journal of the American Chemical Society</i> , 2016, 138, 5511-5514. | 6.6 | 63 |
| 9710 | Regioselective Acylation of Diols and Triols: The Cyanide Effect. <i>Journal of the American Chemical Society</i> , 2016, 138, 6002-6009. | 6.6 | 51 |
| 9711 | Magnetic properties with multiwavelets and DFT: the complete basis set limit achieved. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21145-21161. | 1.3 | 40 |
| 9712 | Quantum chemical exploration on the metabolic mechanisms of caffeine by flavin-containing monooxygenase. <i>Tetrahedron</i> , 2016, 72, 2858-2867. | 1.0 | 8 |
| 9713 | A femtosecond stimulated Raman spectroscopic study on the oxazine ring opening dynamics of structurally-modified indolobenzoxazines. <i>Chemical Physics Letters</i> , 2016, 653, 67-72. | 1.2 | 0 |
| 9714 | Mechanism for Ag (I)-catalyzed decarboxylative chlorination: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 7 |
| 9715 | Optical Excitation in Donor-Pt-Acceptor Complexes: Role of the Structure. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3547-3553. | 1.1 | 11 |
| 9716 | Dimetallaborane analogues of the octaboranes of the type Cp ₂ M ₂ B ₆ H ₁₀ : structural variations with changes in the skeletal electron count. <i>Dalton Transactions</i> , 2016, 45, 9354-9362. | 1.6 | 2 |
| 9717 | DFT investigation of the interaction of gold nanoclusters with poly(amidoamine) PAMAM GO dendrimer. <i>Chemical Physics Letters</i> , 2016, 654, 29-36. | 1.2 | 11 |
| 9718 | Nuclear size effects in vibrational spectra. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15406-15417. | 1.3 | 10 |
| 9719 | Spin and structural features of oxygen dissociation on tetrahedral Ag ₂₀ and Ag ₁₉ Au clusters. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18033-18044. | 1.3 | 15 |
| 9720 | Behavior of the Chemical Potential in Calcite and Magnesite Crystals: A Damped Harmonic Oscillation. <i>Crystal Growth and Design</i> , 2016, 16, 2671-2677. | 1.4 | 11 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9721 | Completing the Heterocubane Family [Cp*AlE] ₄ (E = O, S, Se, and Te) by Selective Oxygenation and Sulfuration of [Cp*Al] ₄ : Density Functional Theory Calculations of [Cp*AlE] ₄ and Reactivity of [Cp*AlO] ₄ toward Hydrolysis. <i>Inorganic Chemistry</i> , 2016, 55, 4915-4923. | 1.9 | 38 |
| 9722 | Design, synthesis and mesomorphic behaviour of a four-ring achiral bent-core liquid crystal in the nematic phase. <i>RSC Advances</i> , 2016, 6, 43069-43079. | 1.7 | 8 |
| 9723 | Structural and Electronic Effects on the Properties of Fe ₂ (dobdc) upon Oxidation with N ₂ O. <i>Inorganic Chemistry</i> , 2016, 55, 4924-4934. | 1.9 | 15 |
| 9724 | Stability and Polaronic Motion of Self-Trapped Holes in Silver Halides: Insight through DFT+U Calculations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 8509-8524. | 1.5 | 9 |
| 9725 | Unsymmetrical PNP-Pincer Type Phosphaalkene Ligands Protected by a Fused-Ring Bulky Eind Group: Synthesis and Applications to Rh(I) and Ir(I) Complexes. <i>Organometallics</i> , 2016, 35, 1526-1533. | 1.1 | 22 |
| 9726 | Î ² -Hematin Crystal Formation: New Insights from Molecular Dynamics Simulations of Small Clusters in Condensed Phase. <i>Crystal Growth and Design</i> , 2016, 16, 2249-2259. | 1.4 | 2 |
| 9727 | Comprehensive <i>Ab Initio</i> Study of Electronic, Optical, and Cohesive Properties of Silicon Quantum Dots of Various Morphologies and Sizes up to Infinity. <i>Journal of Physical Chemistry C</i> , 2016, 120, 11288-11298. | 1.5 | 20 |
| 9728 | Elucidation of the bonding of a near infrared dye to hollow gold nanospheres – a chalcogen tripod. <i>Chemical Science</i> , 2016, 7, 5160-5170. | 3.7 | 19 |
| 9729 | Mechanism, catalysis and predictions of 1,3,2-diazaphospholenes: theoretical insight into highly polarized P–X bonds. <i>Organic Chemistry Frontiers</i> , 2016, 3, 423-433. | 2.3 | 19 |
| 9730 | Noble gas endohedral fullerenes, Ng@C60 (Ng=Ar, Kr): a particular benchmark for assessing the account of non-covalent interactions by density functional theory calculations. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 11 |
| 9731 | Highly efficient heterogeneous catalysts for phenol oxidation: Binuclear pyrrolyl-azine metal complexes encapsulated in NaY zeolite. <i>Microporous and Mesoporous Materials</i> , 2016, 227, 272-280. | 2.2 | 27 |
| 9732 | Quantum Monte Carlo Study of the Reactions of CH with Acrolein: Major and Minor Channels. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3602-3612. | 1.1 | 21 |
| 9733 | MN15: A Kohn–Sham global-hybrid exchange–correlation density functional with broad accuracy for multi-reference and single-reference systems and noncovalent interactions. <i>Chemical Science</i> , 2016, 7, 5032-5051. | 3.7 | 858 |
| 9734 | Distinguishing binding modes of a new phosphonium dye with DNA by surface-enhanced Raman spectroscopy. <i>RSC Advances</i> , 2016, 6, 41927-41936. | 1.7 | 4 |
| 9735 | Correlating Synthetic Methods, Morphology, Atomic-Level Structure, and Catalytic Activity of Sn-Î ² Catalysts. <i>ACS Catalysis</i> , 2016, 6, 4047-4063. | 5.5 | 106 |
| 9736 | Evaluation of structure-reactivity descriptors and biological activity spectra of 4-(6-methoxy-2-naphthyl)-2-butanone using spectroscopic techniques. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 167, 142-156. | 2.0 | 11 |
| 9737 | Bond Fission and Non-Radiative Decay in Iridium(III) Complexes. <i>Inorganic Chemistry</i> , 2016, 55, 5266-5273. | 1.9 | 49 |
| 9738 | Conformational Energy Landscape of the Ritonavir Molecule. <i>Journal of Physical Chemistry B</i> , 2016, 120, 4331-4340. | 1.2 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9739 | Two Equilibria of (N-Methyl-3-pyridinium)chlorocarbene, a Cationic Carbene. <i>Journal of Physical Chemistry A</i> , 2016, 120, 699-708. | 1.1 | 1 |
| 9740 | Excited States of Pt(PF ₃) ₃ and Their Role in Focused Electron Beam Nanofabrication. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10667-10674. | 1.5 | 33 |
| 9741 | Critical Assessment of Time-Dependent Density Functional Theory for Excited States of Open-Shell Systems: II. Doublet-Quartet Transitions. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2517-2527. | 2.3 | 21 |
| 9742 | Influences of S, Se, Te and Po substitutions on structural, electronic and optical properties of hexagonal CuAlO ₂ using GGA and B3LYP functionals. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 14317-14322. | 1.3 | 14 |
| 9743 | Computational approaches to predict binding interactions between mammalian tyrosinases and (S)-(+)-decursin and its analogues as potent inhibitors. <i>RSC Advances</i> , 2016, 6, 46765-46774. | 1.7 | 3 |
| 9744 | Computational Exploration of Rh ^{III} /Rh ^V and Rh ^{III} /Rh ^I Catalysis in Rhodium(III)-Catalyzed C-H Activation Reactions of <i>N</i> -Phenoxyacetamides with Alkynes. <i>Journal of the American Chemical Society</i> , 2016, 138, 6861-6868. | 6.6 | 116 |
| 9745 | Pressure dependent low temperature kinetics for CN + CH ₃ CN: competition between chemical reaction and van der Waals complex formation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15118-15132. | 1.3 | 21 |
| 9746 | A molecular dynamics investigation of the dissociation constants of acetic and oxalic acid in supercritical water. <i>Molecular Physics</i> , 2016, 114, 1915-1921. | 0.8 | 3 |
| 9747 | Electronic structure of p-type perylene monoimide-based donor-acceptor dyes on the nickel oxide (100) surface: a DFT approach. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 14382-14389. | 1.3 | 14 |
| 9748 | Synthesis, optical, and electrochemical properties, and theoretical calculations of BODIPY containing triphenylamine. <i>Heteroatom Chemistry</i> , 2016, 27, 306-315. | 0.4 | 11 |
| 9749 | Tunable adsorption of isocyanides on group 14 (100)-2 Å ⁻¹ surfaces. <i>Applied Surface Science</i> , 2016, 390, 968-973. | 3.1 | 4 |
| 9750 | Mechanistic Insight into the Attachment of Fullerene Derivatives on Crystal Faces of Methylammonium Lead Iodide Based Perovskites. <i>Journal of Physical Chemistry C</i> , 2016, 120, 22426-22432. | 1.5 | 20 |
| 9751 | A density functional theory mechanistic study of thermal decomposition reactions of nitroethyl carboxylates: undermine of pericyclic insight. <i>Heteroatom Chemistry</i> , 2016, 27, 279-289. | 0.4 | 16 |
| 9752 | Computational approaches to the prediction of the redox potentials of iron and copper bioinorganic systems. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1695-1705. | 1.0 | 16 |
| 9753 | Ligand based pharmacophoric modelling and docking of bioactive pyrazolium 3-nitrophthalate (P3NP) on <i>Bacillus subtilis</i> , <i>Aspergillus fumigatus</i> and <i>Aspergillus niger</i> – Computational and Hirshfeld surface analysis. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2016, 163, 352-365. | 1.7 | 29 |
| 9754 | Probing the Reversible Fe ³⁺ -DOPA-Mediated Bridging Interaction in Mussel Foot Protein-1. <i>Journal of Physical Chemistry C</i> , 2016, 120, 21670-21677. | 1.5 | 22 |
| 9755 | Theoretical investigation of the singlet-triplet splittings for carbazole-based thermally activated delayed fluorescence emitters. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26623-26629. | 1.3 | 47 |
| 9756 | Band and bonding characteristics of N ₂ ⁺ ion-doped graphene. <i>RSC Advances</i> , 2016, 6, 84959-84964. | 1.7 | 1 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9757 | The Importance of Methyl Positioning and Tautomeric Equilibria for Imidazole Nucleophilicity. <i>Chemistry - A European Journal</i> , 2016, 22, 15521-15528. | 1.7 | 11 |
| 9758 | Accelerating ab initio molecular dynamics simulations by linear prediction methods. <i>Chemical Physics Letters</i> , 2016, 661, 42-47. | 1.2 | 7 |
| 9759 | Coherent control of long-range photoinduced electron transfer by stimulated X-ray Raman processes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 10001-10006. | 3.3 | 8 |
| 9760 | Implementation of Molecular Gradients for Local Hybrid Density Functionals Using Seminumerical Integration Techniques. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4254-4262. | 2.3 | 33 |
| 9761 | Beyond energies: geometry predictions with the XYG3 type of doubly hybrid density functionals. <i>Chemical Communications</i> , 2016, 52, 13840-13860. | 2.2 | 18 |
| 9762 | Combinatorial Vibration-Mode Assignment for the FTIR Spectrum of Crystalline Melamine: A Strategic Approach toward Theoretical IR Vibrational Calculations of Triazine-Based Compounds. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7427-7433. | 1.1 | 96 |
| 9763 | New copper(II) complexes of the anti-inflammatory drug mefenamic acid: a concerted study including synthesis, physicochemical characterization and their biological evaluation. <i>RSC Advances</i> , 2016, 6, 88546-88558. | 1.7 | 52 |
| 9764 | Structure and electronics properties of novel antimalarial molecules: Comparative study of ferrotriborodiaziquine and ferrodiborotriaziquine with ferroquine using density functional theory. <i>Polyhedron</i> , 2016, 119, 471-482. | 1.0 | 1 |
| 9765 | Exploring Redox States, Doping and Ordering of Electroactive Star-Shaped Oligo(aniline)s. <i>Chemistry - A European Journal</i> , 2016, 22, 16950-16956. | 1.7 | 15 |
| 9766 | Electrochemical and X-ray photoelectron spectroscopic insights into Molybdenum(0) Fischer ethoxycarbene complexes. <i>Electrochimica Acta</i> , 2016, 219, 204-213. | 2.6 | 18 |
| 9767 | Investigation of the identity of the nucleophile initiating the hydrolysis of phosphate esters catalyzed by dinuclear mimics of metallohydrolases. <i>Journal of Inorganic Biochemistry</i> , 2016, 162, 356-365. | 1.5 | 7 |
| 9768 | Theoretical study on the mechanism of palladium-catalyzed sp ² CH bond activation using cyano as a directing group. <i>Journal of Organometallic Chemistry</i> , 2016, 824, 88-98. | 0.8 | 6 |
| 9769 | XPS Fe 2p peaks from iron tris(β ² -diketonates): Electronic effect of the β ² -diketonato ligand. <i>Polyhedron</i> , 2016, 119, 142-150. | 1.0 | 43 |
| 9770 | Benchmarking Electron Densities and Electrostatic Potentials of Proteins from the Three-Partition Frozen Density Embedding Method. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4843-4855. | 2.3 | 11 |
| 9771 | Role of Lanthanide-Ligand bonding in the magnetization relaxation of mononuclear single-ion magnets: A case study on Pyrazole and Carbene ligated Ln(III) (Ln=Tb, Dy, Ho, Er) complexes. <i>Journal of Chemical Sciences</i> , 2016, 128, 1615-1630. | 0.7 | 25 |
| 9772 | The Electrochemical Behavior of Early Metal Metallocene Cp ₂ MCl ₂ Complexes under CO ₂ . <i>Electrochimica Acta</i> , 2016, 218, 110-118. | 2.6 | 7 |
| 9773 | Copper Complexes of New Redox-Active 4,5-Bisguanidino-Substituted Benzodioxole Ligands: Control of the Electronic Structure by Counter-Ligands, Solvent, and Temperature. <i>Chemistry - A European Journal</i> , 2016, 22, 16187-16199. | 1.7 | 38 |
| 9774 | Photophysical Properties of Benzoylgermane and <i>para</i> -Substituted Derivatives: Substituent Effects on Electronic Transitions. <i>ChemPhysChem</i> , 2016, 17, 3460-3469. | 1.0 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9775 | Theoretical Insight into the Mechanisms and Regioselectivity of [4 + 3] and [4 + 1] Annulations of Enals with Azoalkenes Catalyzed by N-Heterocyclic Carbenes. <i>Journal of Organic Chemistry</i> , 2016, 81, 9775-9784. | 1.7 | 41 |
| 9776 | A Dynamic View of Proton-Coupled Electron Transfer in Photocatalytic Water Splitting. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23074-23082. | 1.5 | 23 |
| 9777 | Calculations of the light absorption spectra of porphyrinoid chromophores for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27877-27884. | 1.3 | 8 |
| 9778 | Benchmarking the DFT methodology for assessing antioxidant-related properties: quercetin and edaravone as case studies. <i>Journal of Molecular Modeling</i> , 2016, 22, 250. | 0.8 | 24 |
| 9779 | Experimental and theoretical study of stereochemistry for new pseurotin A3 with an unusual hetero-spirocyclic system. <i>Tetrahedron</i> , 2016, 72, 7194-7199. | 1.0 | 7 |
| 9780 | Unexpected, Latent Radical Reaction of Methane Propagated by Trifluoromethyl Radicals. <i>Journal of Organic Chemistry</i> , 2016, 81, 9820-9825. | 1.7 | 10 |
| 9781 | Different Conformations of 2-Deoxycytidine in the Gas and Solid Phases: Competition between Intra- and Intermolecular Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8199-8210. | 1.1 | 12 |
| 9782 | Pathways for Arene Oxidation in Non-Heme Diiron Enzymes: Lessons from Computational Studies on Benzoyl Coenzyme A Epoxidase. <i>Journal of the American Chemical Society</i> , 2016, 138, 14623-14638. | 6.6 | 11 |
| 9783 | Resolving the origin of the multimode Jahn-Teller effect in metallophthalocyanines. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29122-29130. | 1.3 | 10 |
| 9784 | Remarkable Anion-Dependent Spin-State Switching in Diiron(III) μ_4 -Hydroxo Bisporphyrins: What Role Do Counterions Play?. <i>Chemistry - A European Journal</i> , 2016, 22, 16124-16137. | 1.7 | 30 |
| 9785 | First-Principles Study of Nonradiative Recombination in Silicon Nanocrystals: The Role of Surface Silanol. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23246-23253. | 1.5 | 12 |
| 9786 | Electrocatalytic reduction of carbon dioxide with Mn(terpyridine) carbonyl complexes. <i>Dalton Transactions</i> , 2016, 45, 17179-17186. | 1.6 | 40 |
| 9787 | Aluminum derivative peroxides in the (t-BuO)3Al-2t-BuOOH catalytic system as a source of electron-excited dioxygen: a quantum chemical study on a model. <i>RSC Advances</i> , 2016, 6, 95542-95555. | 1.7 | 1 |
| 9788 | Computational investigation into the gas-phase ozonolysis of the conjugated monoterpene β -phellandrene. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27991-28002. | 1.3 | 14 |
| 9789 | Solvent effects on optical excitations of poly para phenylene ethynylene studied by QM/MM simulations based on many-body Green's functions theory. <i>European Physical Journal: Special Topics</i> , 2016, 225, 1743-1756. | 1.2 | 6 |
| 9790 | Encapsulation of Thiotepa and Altretamine as neurotoxic anticancer drugs in Cucurbit[n]uril (n=7, 8) nanocapsules: A DFT study. <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650056. | 1.8 | 10 |
| 9791 | Synthesis, electronic, and spectral properties of novel geranylated chalcone derivatives: a theoretical and experimental study. <i>Journal of Molecular Modeling</i> , 2016, 22, 253. | 0.8 | 10 |
| 9792 | Optoelectronic properties of naphtho[2, 1-b:6, 5-b']difuran derivatives for photovoltaic application: a computational study. <i>Journal of Molecular Modeling</i> , 2016, 22, 248. | 0.8 | 24 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9793 | Redox Behavior of the <i>S</i> -Adenosylmethionine (SAM)-Binding Fe ⁴ S Cluster in Methylthiotransferase RimO, toward Understanding Dual SAM Activity. <i>Biochemistry</i> , 2016, 55, 5798-5808. | 1.2 | 13 |
| 9794 | Irida- η^2 -ketoimines Derived from Hydrazines To Afford Metallapyrazoles or N ⁺ N Bond Cleavage: A Missing Metallacycle Disclosed by a Theoretical and Experimental Study. <i>Inorganic Chemistry</i> , 2016, 55, 10284-10293. | 1.9 | 1 |
| 9795 | Interactions of Sulfobetaine Zwitterionic Surfactants with Water on Water Surface. <i>Langmuir</i> , 2016, 32, 10905-10911. | 1.6 | 32 |
| 9796 | Catalytic Water-Oxidation Activity of a Weakly Coupled Binuclear Ruthenium Polypyridyl Complex. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 5547-5556. | 1.0 | 18 |
| 9797 | Insights into the spontaneity of hydrogen bond formation between formic acid and phthalimide derivatives. <i>Journal of Molecular Modeling</i> , 2016, 22, 255. | 0.8 | 5 |
| 9798 | Open-ended response theory with polarizable embedding: multiphoton absorption in biomolecular systems. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28339-28352. | 1.3 | 23 |
| 9799 | Construction of copper chains with new fluorescent guanidino-functionalized naphthyridine ligands. <i>Dalton Transactions</i> , 2016, 45, 16966-16983. | 1.6 | 19 |
| 9800 | Electronic and Photophysical Properties of [Re(L)(CO) ₃ (phen)] ⁺ and [Ru(L) ₂ (bpy) ₂] ²⁺ (L = imidazole), Building Units for Long-Range Electron Transfer in Modified Blue Copper Proteins. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6934-6943. | 1.1 | 17 |
| 9801 | Mechanistic Investigation into Olefin Epoxidation with H ₂ O ₂ Catalyzed by Aqua ⁺ -Coordinated Sandwich ⁻ type Polyoxometalates: Role of the Noble Metal and Active Oxygen Position. <i>ChemistryOpen</i> , 2016, 5, 470-476. | 0.9 | 6 |
| 9802 | Application of response surface methodology for exploring β -cyclodextrin effects on the decoloration of spiropyran complexes. <i>Chemical Physics Letters</i> , 2016, 662, 296-305. | 1.2 | 4 |
| 9803 | X-ray and electronic structure of tris(benzoylacetonato- η^2 O, O ²⁻)iron(III). <i>Journal of Molecular Structure</i> , 2016, 1123, 199-205. | 1.8 | 5 |
| 9804 | How Large Should the QM Region Be in QM/MM Calculations? The Case of Catechol <i>O</i> -Methyltransferase. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11381-11394. | 1.2 | 150 |
| 9805 | Raman and IR Spectra of Ice Ih and Ice XI with an Assessment of DFT Methods. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11043-11051. | 1.2 | 18 |
| 9806 | Targeting a Targeted Drug: An Approach Toward Hypoxia ⁺ -Activatable Tyrosine Kinase Inhibitor Prodrugs. <i>ChemMedChem</i> , 2016, 11, 2410-2421. | 1.6 | 18 |
| 9807 | Unexpected Formation and Crystal Structure of the Highly Symmetric Carbanion [C(SiCl ₃) ₃] ⁻ . <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 5028-5035. | 1.0 | 12 |
| 9808 | Refractive indices of organo ⁺ metallic and ⁻ metalloid compounds: A long ⁺ range corrected DFT study. <i>Journal of Computational Chemistry</i> , 2016, 37, 2759-2769. | 1.5 | 4 |
| 9809 | Insights into the Nature and Evolution upon Electrochemical Cycling of Planar Defects in the β -NaMnO ₂ Na-Ion Battery Cathode: An NMR and First-Principles Density Functional Theory Approach. <i>Chemistry of Materials</i> , 2016, 28, 8228-8239. | 3.2 | 58 |
| 9810 | Long-Range Reactivity Modulations in Geranyl Chloride Derivatives. <i>Journal of Organic Chemistry</i> , 2016, 81, 10964-10974. | 1.7 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9811 | Terahertz Phonon Modes of Highly Efficient Electro-optic Phenyltriene OH1 Crystals. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24360-24369. | 1.5 | 12 |
| 9812 | Theoretical Study of the Catalytic Hydrogenation of Alkenes by a Disilaferracyclic Complex: Can the Fe-Si σ -Bond-Assisted Activation of H-H Bonds Allow Development of a Catalysis of Iron?. <i>Journal of Organic Chemistry</i> , 2016, 81, 10900-10911. | 1.7 | 18 |
| 9813 | A Reaction Valley Investigation of the Cycloaddition of 1,3-Dipoles with the Dipolarophiles Ethene and Acetylene: Solution of a Mechanistic Puzzle. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8400-8418. | 1.1 | 21 |
| 9814 | Direct Observation of a Dark State in the Photocycle of a Light-Driven Molecular Motor. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8606-8612. | 1.1 | 36 |
| 9815 | Computational Mechanism for Initiation and Growth of Poly(3-hexylthiophene) Using Palladium η^5 -Heterocyclic Carbene Precatalysts. <i>Macromolecules</i> , 2016, 49, 7632-7641. | 2.2 | 21 |
| 9816 | Synthesis and Isomeric Analysis of Ru(II) Complexes Bearing Pentadentate Scaffolds. <i>Inorganic Chemistry</i> , 2016, 55, 11216-11229. | 1.9 | 17 |
| 9817 | Experimental and DFT Characterization of Halloysite Nanotubes Loaded with Salicylic Acid. <i>Journal of Physical Chemistry C</i> , 2016, 120, 26759-26769. | 1.5 | 29 |
| 9818 | Structural essentials for \hat{I}^2 -N-acetylhexosaminidase inhibition by amides of prolines, pipercolic and azetidine carboxylic acids. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 10371-10385. | 1.5 | 17 |
| 9819 | Thermodynamics of Metal Nanoparticles: Energies and Enthalpies of Formation of Magnesium Clusters and Nanoparticles as Large as 1.3 nm. <i>Journal of Physical Chemistry C</i> , 2016, 120, 26110-26118. | 1.5 | 18 |
| 9820 | Modelling the chemistry of Mn-doped MgO for bulk and (100) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28648-28660. | 1.3 | 11 |
| 9821 | Phosphate Ester Bond Hydrolysis Promoted by Lanthanide-Substituted Keggin-type Polyoxometalates Studied by a Combined Experimental and Density Functional Theory Approach. <i>Inorganic Chemistry</i> , 2016, 55, 9898-9911. | 1.9 | 23 |
| 9822 | Novel non-spherical deltahedra in trirhenaborane structures. <i>New Journal of Chemistry</i> , 2016, 40, 7564-7572. | 1.4 | 4 |
| 9823 | Ammonia-borane dehydrogenation catalyzed by Iron pincer complexes: A concerted metal-ligand cooperation mechanism. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 17208-17215. | 3.8 | 16 |
| 9824 | Fast Time-Dependent Density Functional Theory Calculations of the X-ray Absorption Spectroscopy of Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5018-5025. | 2.3 | 26 |
| 9825 | Quantum Dynamics Simulations of Excited State Energy Transfer in a Zinc-Free-Base Porphyrin Dyad. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8075-8084. | 1.1 | 11 |
| 9826 | Accurate determination of the nuclear quadrupole moment of xenon from the molecular method. <i>Chemical Physics Letters</i> , 2016, 660, 228-232. | 1.2 | 5 |
| 9827 | Influence of dopants Cu, Ga, In, Hg on the electronic structure of Cd _n S _n (n = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10). <i>Journal of Applied Physics</i> , 2016, 119, 155701. | 1.7 | 5 |
| 9828 | Designing intrinsically photostable low band gap polymers: a smart tool combining EPR spectroscopy and DFT calculations. <i>Journal of Materials Chemistry A</i> , 2016, 4, 15647-15654. | 5.2 | 9 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9829 | Diphenylhexatriene membrane probes DPH and TMA-DPH: A comparative molecular dynamics simulation study. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 2647-2661. | 1.4 | 87 |
| 9830 | Getting excited: challenges in quantum-classical studies of excitons in polymeric systems. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30297-30304. | 1.3 | 10 |
| 9831 | The synthesis of a pyridine-N-oxide isophthalamide rotaxane utilizing supplementary amide hydrogen bond interactions. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 7972-7981. | 1.5 | 10 |
| 9832 | Thermochemistry of icosahedral closo-dicboranes: a composite ab initio quantum-chemical perspective. <i>Canadian Journal of Chemistry</i> , 2016, 94, 1082-1089. | 0.6 | 4 |
| 9833 | Synthesis and Single-Molecule Conductance Study of Redox-Active Ruthenium Complexes with Pyridyl and Dihydrobenzo[<i>b</i>]thiophene Anchoring Groups. <i>Chemistry - A European Journal</i> , 2016, 22, 12732-12740. | 1.7 | 26 |
| 9834 | Effects of the acceptor unit in dyes with acceptor-bridge-donor architecture on the electron photo-injection mechanism and aggregation in DSSCs. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24239-24251. | 1.3 | 23 |
| 9835 | DFT 101 and Applications to π -Conjugated Systems. <i>Materials and Energy</i> , 2016, , 19-52. | 2.5 | 0 |
| 9836 | Experimental and Computational Studies of the Single-Molecule Conductance of Ru(II) and Pt(II) <i>trans</i> -Bis(acetylide) Complexes. <i>Organometallics</i> , 2016, 35, 2944-2954. | 1.1 | 49 |
| 9837 | A theoretical study of ruthenium complexes with 2,2-biimidazole-like ligands: structural, optical and emissive properties. <i>Photochemical and Photobiological Sciences</i> , 2016, 15, 1138-1147. | 1.6 | 2 |
| 9838 | Polyhedral cobaltadisenaboranes: nido structures without bridging hydrogens. <i>RSC Advances</i> , 2016, 6, 53635-53642. | 1.7 | 1 |
| 9839 | Facile synthesis, structural evaluation, antimicrobial activity and synergistic effects of novel imidazo[1,2- <i>a</i>]pyridine based organoselenium compounds. <i>European Journal of Medicinal Chemistry</i> , 2016, 123, 916-924. | 2.6 | 81 |
| 9840 | Nonempirical Double-Hybrid Functionals: An Effective Tool for Chemists. <i>Accounts of Chemical Research</i> , 2016, 49, 1503-1513. | 7.6 | 103 |
| 9841 | Electronically Excited States of Borylenes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6332-6341. | 1.1 | 17 |
| 9842 | Theoretical insights into photoinduced proton transfer of 7-hydroxyquinoline via intermolecular hydrogen-bonded wire of mixed methanol and water. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 10 |
| 9843 | Topological Study of Bonding in Aquo and Bis(triazinyl)pyridine Complexes of Trivalent Lanthanides and Actinides: Does Covalency Imply Stability?. <i>Inorganic Chemistry</i> , 2016, 55, 10034-10042. | 1.9 | 41 |
| 9844 | Does the Mechanism of the Garratt-Braverman Cyclization Differ with Substrates? A Computational Study on Bispropargyl Sulfones, Sulfides, Ethers, Amines, and Methanes. <i>Journal of Organic Chemistry</i> , 2016, 81, 7411-7418. | 1.7 | 7 |
| 9845 | Biradical character in the ground state of $[\text{Mn@Si}_{12}]^{+}$: a DFT and CASPT2 study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24006-24014. | 1.3 | 12 |
| 9846 | Analysis of the topology of the electron density and the reactivity descriptors of biomolecules with insecticide activity. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 1 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9847 | Substituent-Modulated Conformation and Supramolecular Assembly of Tetronamides. <i>Crystal Growth and Design</i> , 2016, 16, 5798-5810. | 1.4 | 6 |
| 9848 | Spectroscopic and Computational Study of Acetic Acid and Its Cyclic Dimer in the Near-Infrared Region. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6170-6183. | 1.1 | 44 |
| 9849 | Controlling Visible Light Driven Photoconductivity in Self-Assembled Perylene Bisimide Structures. <i>Journal of Physical Chemistry C</i> , 2016, 120, 18479-18486. | 1.5 | 40 |
| 9850 | Comparative Analysis of Reactant and Product Adsorption Energies in the Selective Oxidative Coupling of Alcohols to Esters on Au(111). <i>Topics in Catalysis</i> , 2016, 59, 1383-1393. | 1.3 | 3 |
| 9851 | Mechanisms for dehydrogenation and hydrogenation of N-heterocycles using PNP-pincer-supported iron catalysts: a density functional study. <i>Dalton Transactions</i> , 2016, 45, 14965-14978. | 1.6 | 24 |
| 9852 | Predicting Pt ¹⁹⁵ NMR chemical shift using new relativistic all-electron basis set. <i>Journal of Computational Chemistry</i> , 2016, 37, 2360-2373. | 1.5 | 24 |
| 9853 | Synthesis, electrochemical and DFT study of octahedral bis(β ² -diketonato)-titanium(IV) complexes. <i>Inorganica Chimica Acta</i> , 2016, 453, 247-256. | 1.2 | 15 |
| 9854 | Photoexcited carriers recombination and trapping in spherical vs faceted TiO ₂ nanoparticles. <i>Nano Energy</i> , 2016, 27, 673-689. | 8.2 | 37 |
| 9855 | Theoretical Modeling of ⁹⁹ Tc NMR Chemical Shifts. <i>Inorganic Chemistry</i> , 2016, 55, 8341-8347. | 1.9 | 10 |
| 9856 | Theoretical study of the cis \leftrightarrow trans isomerization mechanism of a pendant metal-bound azobenzene. <i>RSC Advances</i> , 2016, 6, 79879-79889. | 1.7 | 8 |
| 9857 | The INV24 test set: how well do quantum-chemical methods describe inversion and racemization barriers?. <i>Canadian Journal of Chemistry</i> , 2016, 94, 1133-1143. | 0.6 | 45 |
| 9858 | A Comprehensive Study of Copper Guanidine Quinoline Complexes: Predicting the Activity of Catalysts in ATRP with DFT. <i>Chemistry - A European Journal</i> , 2016, 22, 13550-13562. | 1.7 | 28 |
| 9859 | Indole π -Based Molecular Engineering for Optimizing the Performance of Photoactive Thin Films. <i>Advanced Functional Materials</i> , 2016, 26, 6876-6887. | 7.8 | 18 |
| 9860 | Prefunctionalized Porous Organic Polymers: Effective Supports of Surface Palladium Nanoparticles for the Enhancement of Catalytic Performances in Dehalogenation. <i>Chemistry - A European Journal</i> , 2016, 22, 12533-12541. | 1.7 | 28 |
| 9861 | Investigating the mechanism of the selective hydrogenation reaction of cinnamaldehyde catalyzed by Pt _n clusters. <i>Journal of Molecular Modeling</i> , 2016, 22, 186. | 0.8 | 3 |
| 9862 | Preparation of Capped Octahedral OsHC ₆ Complexes by Sequential Carbon-Directed C-H Bond Activation Reactions. <i>Organometallics</i> , 2016, 35, 2532-2542. | 1.1 | 9 |
| 9863 | Structural features of the carbon π -sulfur chemical bond: a semi-experimental perspective. <i>Canadian Journal of Chemistry</i> , 2016, 94, 1065-1076. | 0.6 | 40 |
| 9864 | Small Atomic Orbital Basis Set First-Principles Quantum Chemical Methods for Large Molecular and Periodic Systems: A Critical Analysis of Error Sources. <i>ChemistryOpen</i> , 2016, 5, 94-109. | 0.9 | 57 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9865 | Alkali Metal Cation versus Proton and Methyl Cation Affinities: Structure and Bonding Mechanism. <i>ChemistryOpen</i> , 2016, 5, 247-253. | 0.9 | 4 |
| 9866 | Electronic Structure Evaluation of an Oxidized Tris(methoxy)-Substituted Ni Salen Complex. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 49-55. | 1.0 | 13 |
| 9867 | Polymer Photocatalysts for Water Splitting: Insights from Computational Modeling. <i>Macromolecular Chemistry and Physics</i> , 2016, 217, 344-353. | 1.1 | 72 |
| 9868 | Effect of Chelate Ring Size in Iron(II) Isothiocyanato Complexes with Tetradentate Tripyridyl-alkylamine Ligands on Spin Crossover Properties. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2016, 642, 85-94. | 0.6 | 5 |
| 9869 | The Initiation Mechanism of Butadiene Polymerization in Aliphatic Hydrocarbons: A Full Mechanistic Approach. <i>Macromolecules</i> , 2016, 49, 5397-5406. | 2.2 | 3 |
| 9870 | Brønsted acidity of protic ionic liquids: a modern ab initio valence bond theory perspective. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26020-26025. | 1.3 | 8 |
| 9871 | Effect of Interporphyrin Distance on Spin State in Diiron(III) Hydroxo Bisporphyrins. <i>Chemistry - A European Journal</i> , 2016, 22, 14585-14597. | 1.7 | 35 |
| 9872 | Computational Discovery of Hydrogen Bond Design Rules for Electrochemical Ion Separation. <i>Chemistry of Materials</i> , 2016, 28, 6207-6218. | 3.2 | 17 |
| 9873 | Density Functional Theory (DFT) and Time Dependent DFT (TDDFT)., 2016, , 155-194. | | 6 |
| 9874 | Mechanistic Insights into the Iridium-Catalyzed Hydrogenations of α,β -Unsaturated Ketones. <i>ChemCatChem</i> , 2016, 8, 3099-3106. | 1.8 | 14 |
| 9875 | Mechanistic aspects of chemo- and regioselectivity in Cp ₂ ZrCl ₂ -catalyzed alkene cycloalumination by AlEt ₃ . <i>Journal of Organometallic Chemistry</i> , 2016, 822, 135-143. | 0.8 | 10 |
| 9876 | Electronic Structure and Optical Properties of Boron Difluoride Dibenzoylmethane Derivatives. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7361-7369. | 1.1 | 20 |
| 9877 | Computational Approach for Studying Optical Properties of DNA Systems in Solution. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5050-5057. | 2.3 | 26 |
| 9878 | Selective hydrogenation of cinnamaldehyde catalyzed by Co-doped Pt clusters: a density functional theoretical study. <i>RSC Advances</i> , 2016, 6, 88277-88286. | 1.7 | 9 |
| 9879 | Computationally designed tandem direct selective oxidation using molecular oxygen as oxidant without coreductant. <i>RSC Advances</i> , 2016, 6, 88189-88215. | 1.7 | 2 |
| 9880 | Ligand-accelerated enantioselective methylene C(sp ³)-H bond activation. <i>Science</i> , 2016, 353, 1023-1027. | 6.0 | 296 |
| 9881 | Kinetic-energy-density dependent semilocal exchange-correlation functionals. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1641-1694. | 1.0 | 78 |
| 9882 | Molecular Insight from DFT Computations and Kinetic Measurements into the Steric Factors Influencing Peptide Bond Hydrolysis Catalyzed by a Dimeric Zr(IV)-Substituted Keggin Type Polyoxometalate. <i>Inorganic Chemistry</i> , 2016, 55, 9316-9328. | 1.9 | 30 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9883 | Fiber enhanced Raman spectroscopic analysis as a novel method for diagnosis and monitoring of diseases related to hyperbilirubinemia and hyperbiliverdinemia. <i>Analyst</i> , The, 2016, 141, 6104-6115. | 1.7 | 48 |
| 9884 | The structure of a one-electron oxidized Mn(III)-bis(phenolate)dipyrin radical complex and oxidation catalysis control via ligand-centered redox activity. <i>Dalton Transactions</i> , 2016, 45, 16325-16334. | 1.6 | 25 |
| 9885 | Chiral dendrigraft polymer for asymmetric synthesis of isoquinuclidines. <i>RSC Advances</i> , 2016, 6, 85643-85658. | 1.7 | 4 |
| 9886 | Multimodel Approach to the Optical Properties of Molecular Dyes in Solution. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4423-4429. | 2.3 | 13 |
| 9887 | Dynamics of Azobenzene Dimer Photoisomerization: Electronic and Steric Effects. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3591-3596. | 2.1 | 42 |
| 9888 | Theoretical study of the interaction between molecular oxygen and tetraaza macrocyclic manganese complexes. <i>Journal of Molecular Modeling</i> , 2016, 22, 217. | 0.8 | 7 |
| 9889 | Dynamic NMR and Quantum-Chemical Study of the Stereochemistry and Stability of the Chiral MoO ₂ (acac) ₂ Complex in Solution. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6677-6687. | 1.1 | 6 |
| 9890 | Reversible Photoreduction as a Trigger for Photoresponsive Gels. <i>Chemistry of Materials</i> , 2016, 28, 6336-6341. | 3.2 | 38 |
| 9891 | Colorimetric detection of hydrogen peroxide using silver nanoparticles with three different morphologies. <i>Analytical Methods</i> , 2016, 8, 6691-6695. | 1.3 | 44 |
| 9892 | Role of Nonbond Interactions in the Glass Transition of Novolac-Type Phenolic Resin: A Molecular Dynamics Study. <i>Industrial & Engineering Chemistry Research</i> , 2016, 55, 9440-9451. | 1.8 | 20 |
| 9893 | Precursor Ion-Induced Ion Aggregation in the Brust-Schiffrin Synthesis of Alkanethiol Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2016, 120, 19837-19847. | 1.5 | 16 |
| 9894 | Does Nature Know Best? Pericyclic Reactions in the <i>Daphniphyllum</i> Alkaloid-Forming Cation Cascade. <i>Organic Letters</i> , 2016, 18, 4482-4484. | 2.4 | 16 |
| 9895 | Vanadium(V) Complexes with Substituted 1,5-bis(2-hydroxybenzaldehyde)carbohydrazones and Their Use As Catalyst Precursors in Oxidation of Cyclohexane. <i>Inorganic Chemistry</i> , 2016, 55, 9187-9203. | 1.9 | 49 |
| 9896 | Synthesis of Co ^{II} -NO ⁺ Complexes and Their Reactivity as a Source of Nitroxyl. <i>Journal of the American Chemical Society</i> , 2016, 138, 12459-12471. | 6.6 | 25 |
| 9897 | Strong Fermi level pinning induces a high rectification ratio and negative differential resistance in hydrogen bonding bridged single cytidine pair junctions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26586-26594. | 1.3 | 14 |
| 9898 | Ultrafast relaxation dynamics of electronically excited piperidine: ionization signatures of Rydberg/valence evolution. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 25070-25079. | 1.3 | 29 |
| 9899 | Multiple Condensation Reactions Involving Pt ^{II} /Pd ^{II} -OH ₂ , Pt ^{II} -NH ₃ , and Cytosine ²⁺ Groups: New Twists in Cisplatin ²⁺ Nucleobase Chemistry. <i>Chemistry - A European Journal</i> , 2016, 22, 13653-13668. | 1.7 | 7 |
| 9900 | Description of excited states in [Re(Imidazole)(CO) ₃ (Phen)] ⁺ including solvent and spin-orbit coupling effects: Density functional theory versus multiconfigurational wavefunction approach. <i>Journal of Computational Chemistry</i> , 2016, 37, 2454-2466. | 1.5 | 30 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9901 | Effect of Complex-Valued Optimal Orbitals on Atomization Energies with the Perdew–Zunger Self-Interaction Correction to Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4296-4302. | 2.3 | 29 |
| 9902 | Iron(III) bis(pyrazol-1-yl)acetate based decanuclear metallacycles: synthesis, structure, magnetic properties and DFT calculations. <i>Dalton Transactions</i> , 2016, 45, 15089-15096. | 1.6 | 10 |
| 9903 | Structure and lattice dynamics of rare-earth ferroborate crystals: Ab initio calculation. <i>Physics of the Solid State</i> , 2016, 58, 1642-1650. | 0.2 | 15 |
| 9904 | Implications of Guanidine Substitution on Copper Complexes as Entatic State Models. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 4731-4743. | 1.0 | 36 |
| 9905 | Photoreduction Mechanism of CO ₂ to CO Catalyzed by a Rhenium(I)–Polyoxometalate Hybrid Compound. <i>ACS Catalysis</i> , 2016, 6, 6422-6428. | 5.5 | 58 |
| 9906 | Spectroscopic properties of BF ₂ complexes of N-(5-phenyl-2-pyrazinyl)pivalamides exhibiting fluorescence in solution and solid state. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 331, 206-214. | 2.0 | 11 |
| 9907 | The electron delocalization range in stretched bonds. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1783-1795. | 1.0 | 6 |
| 9908 | Toward Accurate Modeling of the Effect of Ion-Pair Formation on Solute Redox Potential. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4501-4508. | 2.3 | 22 |
| 9909 | Chiral-Selective Carbon Nanotube Etching with Ammonia: A Quantum Chemical Investigation. <i>Journal of Physical Chemistry C</i> , 2016, 120, 19862-19870. | 1.5 | 7 |
| 9910 | Tetrazine Assists Reduction of Water by Phosphines: Application in the Mitsunobu Reaction. <i>Chemistry - A European Journal</i> , 2016, 22, 13985-13998. | 1.7 | 16 |
| 9911 | Rational Design in Catalysis: A Mechanistic Study of β -Hydride Eliminations in Gold(I) and Gold(III) Complexes Based on Features of the Reaction Valley. <i>Inorganic Chemistry</i> , 2016, 55, 8636-8645. | 1.9 | 40 |
| 9912 | First hyperpolarizability of para-aminoaniline induced by a variety of gold nano particles. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24343-24349. | 1.3 | 3 |
| 9913 | Rational computing of energy levels for organic electronics: the case of 2-benzylidene-1,3-indandiones. <i>RSC Advances</i> , 2016, 6, 85242-85253. | 1.7 | 2 |
| 9914 | Proton-Coupled Electron Transfer in a Strongly Coupled Photosystem II-Inspired Chromophore–Imidazole–Phenol Complex: Stepwise Oxidation and Concerted Reduction. <i>Journal of the American Chemical Society</i> , 2016, 138, 11536-11549. | 6.6 | 66 |
| 9915 | Explicitly correlated frequency-independent second-order Green's function for accurate ionization energies. <i>Journal of Computational Chemistry</i> , 2016, 37, 2447-2453. | 1.5 | 16 |
| 9916 | Characterization of Catechins in Water by Photoemission Yield Spectroscopy in Air. <i>Analytical Sciences</i> , 2016, 32, 577-580. | 0.8 | 2 |
| 9917 | Photoelectron spectra and electronic structure of nitrogen analogues of boron β -diketonates with aromatic substituents. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2016, 213, 32-38. | 0.8 | 3 |
| 9918 | DFT Study of the Mechanisms of Iron-Catalyzed Regioselective Synthesis of β -Aryl Carboxylic Acids from Styrene Derivatives and CO ₂ . <i>Organometallics</i> , 2016, 35, 3932-3938. | 1.1 | 24 |

| # | ARTICLE | IF | CITATIONS |
|------|---|-----|-----------|
| 9919 | Effect of Hydrofluoroether Cosolvent Addition on Li Solvation in Acetonitrile-Based Solvate Electrolytes and Its Influence on S Reduction in a Li-S Battery. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 34360-34371. | 4.0 | 58 |
| 9920 | Structural elucidation and physicochemical properties of mononuclear Uranyl(VI) complexes incorporating dianionic units. <i>Scientific Reports</i> , 2016, 6, 32898. | 1.6 | 15 |
| 9921 | Effect of vanadium valence state on the solution chemistry and the stability of vanadium substituted polyoxometalates. <i>RSC Advances</i> , 2016, 6, 110922-110927. | 1.7 | 2 |
| 9922 | Hybrid functionals with fixed mixing parameter perform no better than PBE for fundamental band gaps of nanoscale materials. <i>Physical Review B</i> , 2016, 94, . | 1.1 | 6 |
| 9923 | A Benefit of Using the IDSCRF- over UFF-Radii Cavities and Why Joint Correlations of NMR Chemical Shifts Can Be Advantageous: Condensed Pyridines as an IEF-PCM/GIAO/DFT Case Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9519-9528. | 1.1 | 7 |
| 9924 | Tetranuclear Lanthanide Complexes Containing a Hydrazone-type Ligand. Dysprosium [2 Å– 2] Gridlike Single-Molecule Magnet and Toric. <i>Inorganic Chemistry</i> , 2016, 55, 12470-12476. | 1.9 | 43 |
| 9925 | Electronic properties of Fe charge transfer complexes – A combined experimental and theoretical approach. <i>Electrochimica Acta</i> , 2016, 216, 339-346. | 2.6 | 31 |
| 9926 | QM/MM calculations on a newly synthesised oxyluciferin substrate: new insights into the conformational effect. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27460-27467. | 1.3 | 22 |
| 9927 | Modification of optoelectronic properties of conjugated oligomers due to donor/acceptor functionalization: DFT study. <i>Chemical Physics</i> , 2016, 481, 133-143. | 0.9 | 7 |
| 9928 | Catalytic, Vicinal Difluorination of Olefins: Creating a Hybrid, Chiral Bioisostere of the Trifluoromethyl and Ethyl Groups. <i>ACS Catalysis</i> , 2016, 6, 7167-7173. | 5.5 | 78 |
| 9929 | Origins of Selectivity and General Model for Chiral Phosphoric Acid-Catalyzed Oxetane Desymmetrizations. <i>Journal of the American Chemical Society</i> , 2016, 138, 12356-12359. | 6.6 | 50 |
| 9930 | Effects of chemical substitutions on the properties of azacalixpyrins: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27308-27316. | 1.3 | 8 |
| 9931 | Adsorption of 2,4-D on magnetic graphene and mechanism study. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2016, 509, 367-375. | 2.3 | 65 |
| 9932 | Ionization dynamics of orbitals and high-harmonic generation of N ₂ and CO molecules at the various XC potentials by TD-DFT. <i>Computational and Theoretical Chemistry</i> , 2016, 1095, 104-111. | 1.1 | 11 |
| 9933 | Range-Separation Parameter in Tuned Exchange-Correlation Functionals: Successive Ionizations and the Fukui Function. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4879-4884. | 2.3 | 11 |
| 9934 | A comparison of MOP-phosphonite ligands and their applications in Rh(<i>sc</i>)- and Pd(<i>sc</i>)-catalysed asymmetric transformations. <i>Dalton Transactions</i> , 2016, 45, 15660-15670. | 1.6 | 8 |
| 9935 | Quantitative Assessment of Aromaticity and Antiaromaticity Utilizing Vibrational Spectroscopy. <i>Journal of Organic Chemistry</i> , 2016, 81, 9669-9686. | 1.7 | 56 |
| 9936 | Partition coefficients for the SAMPL5 challenge using transfer free energies. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 1129-1138. | 1.3 | 19 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9937 | A Dynamic Equilibrium of Three Hydrogen-Bond Conformers Explains the NMR Spectrum of the Active Site of Photoactive Yellow Protein. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5170-5178. | 2.3 | 3 |
| 9938 | Photochemistry of Dithiocarbamate $\text{Cu}(\text{S}_2\text{CNEt}_2)_2$ Complex in CHCl_3 . Transient Species and TD-DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7873-7880. | 1.1 | 7 |
| 9939 | Electrochemical and Spectroscopic Study of Mononuclear Ruthenium Water Oxidation Catalysts: A Combined Experimental and Theoretical Investigation. <i>ACS Catalysis</i> , 2016, 6, 7340-7349. | 5.5 | 15 |
| 9940 | Quantum molecular motion in the mixed ion-radical complex, $[(\text{H}_2\text{O})(\text{H}_2\text{S})]^{+}$. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27450-27459. | 1.3 | 5 |
| 9941 | Facile synthesis of benzothiadiazole-based chromophores for enhanced performance of second-order nonlinear optical materials. <i>Journal of Materials Chemistry C</i> , 2016, 4, 9094-9102. | 2.7 | 20 |
| 9942 | Tailoring the electronic properties among oxoarsine, arsinoyl and arsine oxide isomers: the simplest molecular systems with an arsenic-oxygen bond. <i>RSC Advances</i> , 2016, 6, 90760-90770. | 1.7 | 9 |
| 9943 | Theoretical study of the thermochemistry of chlorine oxyfluorides. <i>Chemical Physics Letters</i> , 2016, 663, 16-20. | 1.2 | 1 |
| 9944 | A mechanistic approach to explore novel HDAC1 inhibitor using pharmacophore modeling, 3D-QSAR analysis, molecular docking, density functional and molecular dynamics simulation study. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 70, 54-69. | 1.3 | 32 |
| 9945 | Family of $\text{MnIII}_4\text{LnIII}_2$ ($\text{LnIII} = \text{SmIII}, \text{GdIII}, \text{DyIII}$) coordination clusters: Experimental and theoretical investigations. <i>Polyhedron</i> , 2016, 119, 202-215. | 1.0 | 8 |
| 9946 | Theoretical and experimental study of the nickel-catalyzed isomerization of 2-Methyl-3-butenenitrile and the effect of a Lewis acid. <i>Journal of Organometallic Chemistry</i> , 2016, 822, 29-38. | 0.8 | 4 |
| 9947 | Modelling fluorescence lifetimes with TD-DFT: a case study with syn-bimanes. <i>RSC Advances</i> , 2016, 6, 87237-87245. | 1.7 | 13 |
| 9948 | Mechanistic Insights of a Selective C-H Alkylation of Alkenes by a Ru-based Catalyst and Alcohols. <i>ChemistrySelect</i> , 2016, 1, 4218-4228. | 0.7 | 3 |
| 9949 | The Electronic Structure of $[\text{Mn}(\text{V})\text{O}]$: What is the Connection between Oxyl Radical Character, Physical Oxidation State, and Reactivity?. <i>ACS Catalysis</i> , 2016, 6, 7202-7216. | 5.5 | 28 |
| 9950 | Judicious Ligand Design in Ruthenium Polypyridyl CO_2 Reduction Catalysts to Enhance Reactivity by Steric and Electronic Effects. <i>Chemistry - A European Journal</i> , 2016, 22, 14870-14880. | 1.7 | 35 |
| 9951 | Two new sesterterpenoids, terretonins H and I, from the marine-derived fungus <i>Aspergillus ustus</i> . <i>Phytochemistry Letters</i> , 2016, 17, 135-139. | 0.6 | 20 |
| 9952 | Deleterious Effects of Exact Exchange Functionals on Predictions of Molecular Conductance. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3431-3435. | 2.3 | 10 |
| 9953 | Effect of surface modification of poly(l-lactide-co- μ -caprolactone) membranes by low-pressure plasma on support cell biocompatibility. <i>Surface and Coatings Technology</i> , 2016, 306, 328-335. | 2.2 | 19 |
| 9954 | Investigation on the neutral and anionic $\text{B}_x\text{Al}_y\text{H}_2$ ($x + y = 7, 8, 9$) clusters using density functional theory combined with photoelectron spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 23296-23303. | 1.3 | 3 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9955 | Joined X-ray, spectroscopic and theoretical study of potential antibacterial cyano group containing fluoroquinolone drugs precursors with the focus on the conformational behavior. Journal of Molecular Structure, 2016, 1125, 736-750. | 1.8 | 4 |
| 9956 | Interaction of Boron-11 Nitrogen Doped Benzene Isomers with Water. Journal of Physical Chemistry A, 2016, 120, 6287-6302. | 1.1 | 15 |
| 9957 | Surface directed reversible imidazole ligation to nickel(II) octaethylporphyrin at the solution/solid interface: a single molecule level study. Physical Chemistry Chemical Physics, 2016, 18, 20819-20829. | 1.3 | 23 |
| 9958 | Synthesis and electronic structure determination of uranium(VI) ligand radical complexes. Dalton Transactions, 2016, 45, 12576-12586. | 1.6 | 30 |
| 9959 | Study on mechanism of isomerization between ammonium thiocyanate and thiourea. Journal of Molecular Structure, 2016, 1125, 643-648. | 1.8 | 8 |
| 9960 | Complete analytic anharmonic hyper-Raman scattering spectra. Physical Chemistry Chemical Physics, 2016, 18, 22331-22342. | 1.3 | 5 |
| 9961 | molSimplify: A toolkit for automating discovery in inorganic chemistry. Journal of Computational Chemistry, 2016, 37, 2106-2117. | 1.5 | 127 |
| 9962 | Employing Range Separation on the meta-GGA Rung: New Functional Suitable for Both Covalent and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2016, 12, 3662-3673. | 2.3 | 10 |
| 9963 | Quantitative Index of the Relative Ease of Formation and σ -Bonding Strength of N-Heterocyclic Carbenes. Journal of Organic Chemistry, 2016, 81, 10295-10301. | 1.7 | 17 |
| 9964 | Benchmark fragment-based ^1H , ^{13}C , ^{15}N and ^{17}O chemical shift predictions in molecular crystals. Physical Chemistry Chemical Physics, 2016, 18, 21686-21709. | 1.3 | 94 |
| 9965 | A dinuclear [(p-cym)Ru(II)Cl] ₂ (1/4-bpytz) TM complex bridged by a radical anion: synthesis, spectroelectrochemical, EPR and theoretical investigation (bpytz) Tj ETQ0 0 0 rgBT /Overlock 10 T 12532-12538. | 1.6 | 18 |
| 9966 | Correlation effects and orbital magnetism of Co clusters. Physical Review B, 2016, 93, . | 1.1 | 12 |
| 9967 | Electronic and optical properties of hexathiapentacene in the gas and crystal phases. Physical Review B, 2016, 93, . | 1.1 | 29 |
| 9968 | Photochemistry of [Ru(pytz)(btz) ₂] ²⁺ and Characterization of a $^1\text{Ru}^{\text{I}}$ -btz Ligand-Loss Intermediate. Inorganic Chemistry, 2016, 55, 7787-7796. | 1.9 | 23 |
| 9969 | The Important Role of the Hydroxyl Group on the Conformational Adaptability in Bis(l-threoninato)copper(II) Compared to Bis(l-allo-threoninato)copper(II): Quantum Chemical Study. Inorganic Chemistry, 2016, 55, 7694-7708. | 1.9 | 7 |
| 9970 | Dissociative electron transfer in polychlorinated aromatics. Reduction potentials from convolution analysis and quantum chemical calculations. Physical Chemistry Chemical Physics, 2016, 18, 22573-22582. | 1.3 | 20 |
| 9971 | Dynamical screening in correlated electron systems—from lattice models to realistic materials. Journal of Physics Condensed Matter, 2016, 28, 383001. | 0.7 | 50 |
| 9972 | A Quantitative Description of the σ -Donor and π -Acceptor Properties of Substituted Phenanthrolines. European Journal of Inorganic Chemistry, 2016, 2016, 3829-3837. | 1.0 | 17 |

| # | ARTICLE | IF | CITATIONS |
|------|--|-----|-----------|
| 9973 | Ferrocene in oil/water interfaces: An electrochemical approach. <i>Electrochimica Acta</i> , 2016, 212, 195-200. | 2.6 | 1 |
| 9974 | Dinuclear metal(μ -acetato) complexes based on bicompartamental 4-chlorophenolate: syntheses, structures, magnetic properties, DNA interactions and phosphodiester hydrolysis. <i>Dalton Transactions</i> , 2016, 45, 12933-12950. | 1.6 | 45 |
| 9975 | A Multifunctional Mn(II) Phosphonate for Rapid Separation of Methyl Orange and Electron-Transfer Photochromism. <i>Chemistry - A European Journal</i> , 2016, 22, 11652-11659. | 1.7 | 34 |
| 9976 | [Al ₂ O ₄] ⁺ , a Benchmark Gas-Phase Class II Mixed-Valence Radical Anion for the Evaluation of Quantum-Chemical Methods. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3796-3806. | 2.3 | 20 |
| 9977 | Extended diketopyrrolopyrrole porphyrin arrays: one- and two-photon photophysical investigations and theoretical studies. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21954-21965. | 1.3 | 30 |
| 9978 | Interactions of Pt nanoparticles with molecular components in polymer electrolyte membrane fuel cells: multi-scale modeling approach. <i>RSC Advances</i> , 2016, 6, 69670-69676. | 1.7 | 31 |
| 9979 | Theoretical investigation of the broad one-photon absorption line-shape of a flexible symmetric carbazole derivative. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22889-22905. | 1.3 | 14 |
| 9980 | Analysis of the Molecules Structure and Vertical Electron Affinity of Organic Gas Impact on Electric Strength. <i>Plasma Science and Technology</i> , 2016, 18, 554-559. | 0.7 | 14 |
| 9981 | Group 14 Dithienometalole-Linked Ethynylene-Conjugated Porphyrin Dimers. <i>Inorganic Chemistry</i> , 2016, 55, 7432-7441. | 1.9 | 20 |
| 9982 | Quantum chemical mass spectrometry: ab initio prediction of electron ionization mass spectra and identification of new fragmentation pathways. <i>Journal of Mass Spectrometry</i> , 2016, 51, 602-614. | 0.7 | 22 |
| 9983 | The role of OH \cdots O and CH \cdots O hydrogen bonds and H \cdots H interactions in ethanol/methanol-water heterohexamers. <i>Journal of Molecular Modeling</i> , 2016, 22, 181. | 0.8 | 6 |
| 9984 | Excited states in large molecular systems through polarizable embedding. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20234-20250. | 1.3 | 78 |
| 9985 | The XYG3 type of doubly hybrid density functionals. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016, 6, 721-747. | 6.2 | 52 |
| 9986 | Effect of Molecular Interactions on Electron-Transfer and Antioxidant Activity of Bis(alkanol)selenides: A Radiation Chemical Study. <i>Chemistry - A European Journal</i> , 2016, 22, 12189-12198. | 1.7 | 11 |
| 9987 | Revisiting alternative pathways in the Fischer-Tropsch process: Accurate density functional theory calculations on μ -magnetic Ru ₁₂ clusters. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1451-1458. | 1.0 | 2 |
| 9988 | Synthesis, anticancer activity and photostability of novel 3-ethyl-2-mercapto-thieno[2,3-d]pyrimidin-4(1H)-one. <i>Journal of Physical Chemistry C</i> , 2016, 120, 17501-17513. | 2.6 | 32 |
| 9989 | Isomeric and Isostructural Oligothiopyranes: Structurally Similar, Physicochemically Different: The Effect of Interplay between H \cdots C(=O), S \cdots C(=O), and Chalcogen S \cdots S Interactions. <i>Crystal Growth and Design</i> , 2016, 16, 4292-4308. | 1.4 | 12 |
| 9990 | Electronic Structure of Small Surfactants: A Continuum Solvation Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 17501-17513. | 1.5 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 9991 | Synthesis of a labile sulfur-centred ligand, [S(H)C(PPh ₂) ₂] ⁺ : structural diversity in lithium(i), zinc(ii) and nickel(ii) complexes. Dalton Transactions, 2016, 45, 12691-12701. | 1.6 | 3 |
| 9992 | Benchmarking the pseudopotential and fixed-node approximations in diffusion Monte Carlo calculations of molecules and solids. Physical Review B, 2016, 93, . | 1.1 | 23 |
| 9993 | Simulating atomic force microscope images with density functional theory: The role of nonclassical contributions to the force. Physical Review B, 2016, 94, . | 1.1 | 2 |
| 9994 | Systematic spatial and stoichiometric screening towards understanding the surface of ultrasmall oxygenated silicon nanocrystal. Applied Surface Science, 2016, 387, 771-778. | 3.1 | 1 |
| 9995 | Dimension and bridging ligand effects on Mo-mediated catalytic transformation of dinitrogen to ammonia: Chain-like extended models of Nishibayashi's catalyst. Computational and Theoretical Chemistry, 2016, 1095, 134-141. | 1.1 | 3 |
| 9996 | In silico study of amphiphilic nanotubes based on cyclic peptides in polar and non-polar solvent. Journal of Molecular Modeling, 2016, 22, 264. | 0.8 | 5 |
| 9997 | Characterization of tenofovir, tenofovir disoproxil fumarate and emtricitabine in aqueous solutions containing sodium ions using ESI-MS, NMR and Ab initio calculations. International Journal of Mass Spectrometry, 2016, 410, 1-11. | 0.7 | 2 |
| 9998 | Accelerating Real-Time Time-Dependent Density Functional Theory with a Nonrecursive Chebyshev Expansion of the Quantum Propagator. Journal of Chemical Theory and Computation, 2016, 12, 5333-5338. | 2.3 | 18 |
| 9999 | Effective Fully Polarizable QM/MM Approach To Model Vibrational Circular Dichroism Spectra of Systems in Aqueous Solution. Journal of Chemical Theory and Computation, 2016, 12, 5483-5492. | 2.3 | 52 |
| 10000 | Spin-Forbidden Transitions between Electronic States in the Active Site of Rubredoxin. Journal of Physical Chemistry A, 2016, 120, 8691-8698. | 1.1 | 7 |
| 10001 | Performance of Hybrid DFT Compared to MP2 Methods in Calculating Nonlinear Optical Properties of Divinylpyrene Derivative Molecules. Journal of Physical Chemistry A, 2016, 120, 8843-8852. | 1.1 | 43 |
| 10002 | How Static Disorder Mimics Decoherence in Anisotropy Pump-Probe Experiments on Purple-Bacteria Light Harvesting Complexes. Journal of Physical Chemistry B, 2016, 120, 11449-11463. | 1.2 | 9 |
| 10003 | Computational Study of First-Row Transition Metals Supported on MOF NU-1000 for Catalytic Acceptorless Alcohol Dehydrogenation. Journal of Physical Chemistry C, 2016, 120, 24697-24705. | 1.5 | 40 |
| 10004 | Metal-free photochemical silylations and transfer hydrogenations of benzenoid hydrocarbons and graphene. Nature Communications, 2016, 7, 12962. | 5.8 | 58 |
| 10005 | Formation of the prebiotic molecule NH ₂ CHO on astronomical amorphous solid water surfaces: accurate tunneling rate calculations. Physical Chemistry Chemical Physics, 2016, 18, 29278-29285. | 1.3 | 67 |
| 10006 | Origins of Stereoselectivity of Chiral Vicinal Diamine-Catalyzed Aldol Reactions. Journal of Organic Chemistry, 2016, 81, 12408-12415. | 1.7 | 12 |
| 10007 | Electronic and optical absorption properties of the derivatives of 1,3,4-Oxadiazole. Chemical Data Collections, 2016, 5-6, 88-95. | 1.1 | 4 |
| 10008 | p-Terphenyl-based di-o-carboranyl compounds: Alteration of electronic transition state by terminal phenyl groups. Journal of Organometallic Chemistry, 2016, 825-826, 69-74. | 0.8 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 10009 | Synthesis, Structure, and Local Molecular Dynamics for Crystalline Rotors Based on Hecogenin/Botogenin Steroidal Frameworks. <i>Crystal Growth and Design</i> , 2016, 16, 5698-5709. | 1.4 | 12 |
| 10010 | Where Does the Density Localize? Convergent Behavior for Global Hybrids, Range Separation, and DFT+U. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5931-5945. | 2.3 | 65 |
| 10011 | Size and Site Dependence of the Catalytic Activity of Iridium Clusters toward Ethane Dehydrogenation. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9500-9508. | 1.1 | 6 |
| 10012 | Experimental and theoretical study of I ₂ -catalyzed dialkenyl oxindoles synthesis from isatins and Î±-cyano ketene ethylene dithioacetate. <i>Synthetic Communications</i> , 2016, 46, 1924-1931. | 1.1 | 2 |
| 10013 | Nearsightedness of Oxygen-Containing Functional Groups. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9579-9587. | 1.1 | 2 |
| 10014 | Probing Electronic Wave Functions of Sodium-Doped Clusters: Dyson Orbitals, Anisotropy Parameters, and Ionization Cross-Sections. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9841-9856. | 1.1 | 20 |
| 10015 | A curious interplay in the films of N-heterocyclic carbene PtII complexes upon deposition of alkali metals. <i>Scientific Reports</i> , 2016, 6, 25548. | 1.6 | 5 |
| 10016 | Acquiring a record barrier height for magnetization reversal in lanthanide encapsulated fullerene molecules using DFT and ab initio calculations. <i>Chemical Communications</i> , 2016, 52, 14047-14050. | 2.2 | 45 |
| 10017 | Time-dependent density-functional description of nuclear dynamics. <i>Reviews of Modern Physics</i> , 2016, 88, . | 16.4 | 185 |
| 10018 | A Low-Temperature, Solution-Processable Organic Electron-Transporting Layer Based on Planar Coronene for High-Performance Conventional Perovskite Solar Cells. <i>Advanced Materials</i> , 2016, 28, 10786-10793. | 11.1 | 102 |
| 10019 | Low-lying electronic excitations of a water-soluble BODIPY: from the gas phase to the solvated molecule. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 4 |
| 10020 | Double helicenes. <i>Chemical Physics Letters</i> , 2016, 666, 13-18. | 1.2 | 3 |
| 10021 | Restricted-Open-Shell G4(MP2)-Type Procedures. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9299-9304. | 1.1 | 19 |
| 10022 | Chemical and Radiation Stability of Ionic Liquids: A Computational Screening Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27757-27767. | 1.5 | 45 |
| 10023 | First-Principle Calculations of the Band Shapes of Singlet-Triplet Transitions. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24605-24614. | 1.5 | 8 |
| 10024 | Dehalogenation of chloroalkanes by nickel(<i>ii</i>) porphyrin derivatives, a computational study. <i>Dalton Transactions</i> , 2016, 45, 16869-16877. | 1.6 | 12 |
| 10025 | Solvent-induced structural diversity in tetranuclear Ni(<i>ii</i>) Schiff-base complexes: the first Ni ₄ single-molecule magnet with a defective cubane-like topology. <i>Dalton Transactions</i> , 2016, 45, 18622-18634. | 1.6 | 49 |
| 10026 | Strategy for Improved Photoconversion Efficiency in Thin Photoelectrode Films by Controlling Î€-Spacer Dihedral Angle. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24655-24666. | 1.5 | 24 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 10027 | Under what conditions does (SiO) _N nucleation occur? A bottom-up kinetic modelling evaluation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26913-26922. | 1.3 | 37 |
| 10028 | Synthesis and crystal structure of nitrosoruthenium complexes cis-[Ru(NO)Py ₂ Cl ₂ (OH)] and cis-[Ru(NO)Py ₂ Cl ₂ (H ₂ O)]Cl. Photoinduced transformations of cis-[Ru(NO)Py ₂ Cl ₂ (OH)]. <i>New Journal of Chemistry</i> , 2016, 40, 10267-10273. | 1.4 | 10 |
| 10029 | Comprehensive structure–function correlation of photoactive ionic π -conjugated supermolecular assemblies: an experimental and computational study. <i>Journal of Materials Chemistry C</i> , 2016, 4, 10223-10239. | 2.7 | 32 |
| 10030 | Absolute Configuration Determination of 2,3-Dihydro-1 <i>H</i> ,5 <i>H</i> -pyrazolo[1,2- <i>a</i>]pyrazoles Using Chiroptical Methods at Different Wavelengths. <i>Journal of Organic Chemistry</i> , 2016, 81, 11802-11812. | 1.7 | 10 |
| 10031 | Symmetry-Adapted Perturbation Theory Energy Analysis of Alkyl Fluorine–Aromatic Interactions in Torsion Balance Systems. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9292-9298. | 1.1 | 10 |
| 10032 | Atropisomerism in 3-arylthiazolidine-2-thiones. A combined dynamic NMR and dynamic HPLC study. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 11137-11147. | 1.5 | 19 |
| 10033 | Accelerated Broadband Spectra Using Transition Dipole Decomposition and Pad $\hat{\circ}$ Approximants. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3741-3750. | 2.3 | 86 |
| 10034 | Impact of Selected LiPF ₆ Hydrolysis Products on the High Voltage Stability of Lithium-Ion Battery Cells. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 30871-30878. | 4.0 | 66 |
| 10035 | Structure, lattice dynamics, and exchange interaction in Lu ₂ V ₂ O ₇ , Y ₂ V ₂ O ₇ : an ab initio approach. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2016, 121, 544-548. | 0.2 | 2 |
| 10036 | Theoretical study of the optical and charge transport properties of π -conjugated three-coordinate organoboron compounds as organic light-emitting diodes materials. <i>RSC Advances</i> , 2016, 6, 108209-108216. | 1.7 | 4 |
| 10037 | Electronic, optical and vibrational features of BiVO ₄ nanostructures investigated by first-principles calculations. <i>RSC Advances</i> , 2016, 6, 110695-110705. | 1.7 | 12 |
| 10038 | Assessment of quantum chemical methods for the calculation of homolytic N–F bond dissociation energies. <i>Chemical Data Collections</i> , 2016, 5-6, 28-35. | 1.1 | 5 |
| 10039 | Kinetics and Thermodynamics of Reversible Thiol Additions to Mono- and Diactivated Michael Acceptors: Implications for the Design of Drugs That Bind Covalently to Cysteines. <i>Journal of Organic Chemistry</i> , 2016, 81, 11726-11733. | 1.7 | 106 |
| 10040 | Structure of N ² -(adamantan-2-ylidene)benzohydrazide, a potential antibacterial agent, in solution: Molecular dynamics simulations, quantum chemical calculations and Ultraviolet–visible spectroscopy studies. <i>Journal of Chemical Sciences</i> , 2016, 128, 1933-1942. | 0.7 | 4 |
| 10041 | Computational study on the synthesis of 1-phenyl-3,4-dihydro- β -carbolone: T ₃ P ⁺ -promoted one-pot formation from tryptamine vs. POCl ₃ -mediated ring closure of Nb-benzoyltryptamine. The first DFT investigation of the Bischler-Napieralski reaction. <i>Computational and Theoretical Chemistry</i> , 2016, 1097, 48-60. | 1.1 | 2 |
| 10042 | Theoretical Calculation of p <i>K</i> _a ™s of Selenols in Aqueous Solution Using an Implicit Solvation Model and Explicit Water Molecules. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8916-8922. | 1.1 | 38 |
| 10043 | Rational design of redox mediators for advanced Li–O ₂ batteries. <i>Nature Energy</i> , 2016, 1, . | 19.8 | 321 |
| 10044 | Exploring short intramolecular interactions in alkylaromatic substrates. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29616-29628. | 1.3 | 11 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10045 | The mechanism of Claisen rearrangement of allyl phenyl ether from the perspective of topological analysis of the ELF. <i>New Journal of Chemistry</i> , 2016, 40, 8717-8726. | 1.4 | 18 |
| 10046 | Electronic excitation and injection of Ru-N3 dye anchored to TiO ₂ surface. <i>Computational and Theoretical Chemistry</i> , 2016, 1097, 8-14. | 1.1 | 1 |
| 10047 | A theoretical investigation of the Zn-doping influence on structural and electronic properties of BaTiO ₃ . <i>Solid State Ionics</i> , 2016, 297, 36-42. | 1.3 | 19 |
| 10048 | Switching of Adsorption Properties in a Zwitterionic Metal-Organic Framework Triggered by Photogenerated Radical Triplets. <i>Chemistry of Materials</i> , 2016, 28, 7825-7832. | 3.2 | 65 |
| 10049 | Exploring the validity of the Glidewell-Lloyd extension of Clar's π -sextet rule: assessment from polycyclic conjugated hydrocarbons. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 24 |
| 10050 | Structure and stability of neutral Al-Mg nanoclusters up to 55 atoms. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31579-31585. | 1.3 | 10 |
| 10051 | Revealing the underlying absorption and emission mechanism of nitrogen doped graphene quantum dots. <i>Nanoscale</i> , 2016, 8, 19376-19382. | 2.8 | 74 |
| 10052 | 2,6-diformyl-4-tert-butylphenol bis-ferrocenoylhydrazone and binuclear copper(II) complexes on its basis. <i>Russian Journal of General Chemistry</i> , 2016, 86, 2075-2080. | 0.3 | 2 |
| 10053 | A computational investigation into the catalytic activity of a diselenolene sulfite oxidase biomimetic complex. <i>Canadian Journal of Chemistry</i> , 2016, 94, 1127-1132. | 0.6 | 5 |
| 10054 | Exchange interaction in pyrochlore vanadates Lu ₂ V ₂ O ₇ and Y ₂ V ₂ O ₇ : Ab initio approach. <i>Physics of the Solid State</i> , 2016, 58, 1989-1994. | 0.2 | 1 |
| 10055 | Investigation of N-Heterocyclic Carbene-Supported Group 12 Triflates as Pre-catalysts for Hydrosilylation/Borylation. <i>Chemistry - A European Journal</i> , 2016, 22, 18236-18246. | 1.7 | 25 |
| 10056 | A Soft Grip: Magnesium Complexes with a Phosphine-Modified Phosphonium Dylidic Lewis Base. <i>Chemistry - A European Journal</i> , 2016, 22, 17425-17435. | 1.7 | 20 |
| 10057 | A stereodynamic phosphoramidite ligand derived from 3,3'-functionalized <i>ortho</i> -biphenol and its rhodium(I) complex. <i>Chirality</i> , 2016, 28, 744-748. | 1.3 | 8 |
| 10058 | Basis set effects on the geometry of C ₉₆ H ₂₄ . <i>Chemical Physics Letters</i> , 2016, 665, 100-104. | 1.2 | 7 |
| 10059 | Different QM/MM Approaches To Elucidate Enzymatic Reactions: Case Study on ppGalNAcT2. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 6062-6076. | 2.3 | 11 |
| 10060 | Interactions between 2,4-bis-pteridine-1,5-benzodiazepine and group 12 dihalides: synthesis, spectral and XRD structural studies and theoretical calculations. <i>Dalton Transactions</i> , 2016, 45, 17896-17909. | 1.6 | 5 |
| 10061 | An adamantane-based disubstituted binding motif with picomolar dissociation constants for cucurbit[n]urils in water and related quaternary assemblies. <i>RSC Advances</i> , 2016, 6, 105146-105153. | 1.7 | 11 |
| 10062 | Tetracarboranes: nido structures without bridging hydrogens. <i>Dalton Transactions</i> , 2016, 45, 18541-18551. | 1.6 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10063 | CO ₂ capture in amine solutions: modelling and simulations with non-empirical methods. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 503003. | 0.7 | 8 |
| 10064 | The Heaviest Possible Ternary Trihalogen Species, IAtBr ⁺ , Evidenced in Aqueous Solution: An Experimental Performance Driven by Computations. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 15369-15372. | 7.2 | 15 |
| 10065 | Tetra- and Pentacationic Electrophiles and Their Chemistry. <i>Journal of Organic Chemistry</i> , 2016, 81, 11758-11765. | 1.7 | 14 |
| 10066 | Ab Initio Thermodynamic and Thermophysical Properties of Sodium Metasilicate, Na ₂ SiO ₃ , and Their Electron-Density and Electron-Pair-Density Counterparts. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8881-8895. | 1.1 | 20 |
| 10067 | Two-Photon-Excited Fluorescence-Encoded Infrared Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9178-9187. | 1.1 | 17 |
| 10068 | Toward Accurate Adsorption Energetics on Clay Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 26402-26413. | 1.5 | 30 |
| 10069 | DFT analysis of the electronic structure of Fe(IV) species active in nitrene transfer catalysis: influence of the coordination sphere. <i>Journal of Molecular Modeling</i> , 2016, 22, 278. | 0.8 | 9 |
| 10070 | Characterization of polar organosulfates in secondary organic aerosol from the unsaturated aldehydes 2-pentenal, 2-hexenal, and 3-hexenal. <i>Atmospheric Chemistry and Physics</i> , 2016, 16, 7135-7148. | 1.9 | 41 |
| 10072 | Peptide Reactivity of Isothiocyanates – Implications for Skin Allergy. <i>Scientific Reports</i> , 2016, 6, 21203. | 1.6 | 22 |
| 10073 | Generalization of Dielectric-Dependent Hybrid Functionals to Finite Systems. <i>Physical Review X</i> , 2016, 6, . | 2.8 | 49 |
| 10074 | Computing dispersive, polarizable, and electrostatic shifts of excitation energy in supramolecular systems: PTCDI crystal. <i>Journal of Chemical Physics</i> , 2016, 145, 094109. | 1.2 | 3 |
| 10075 | Comparison of experimental and DFT-calculated NMR chemical shifts of 2-amino and 2-hydroxyl substituted phenyl benzimidazoles, benzoxazoles and benzothiazoles in four solvents using the IEF-PCM solvation model. <i>Magnetic Resonance in Chemistry</i> , 2016, 54, 298-307. | 1.1 | 8 |
| 10076 | An experimental and theoretical study on the preparation of 4,4'-methylene-bis(N,N -dimethylaniline) in ionic liquid. <i>Journal of Physical Organic Chemistry</i> , 2016, 29, 276-280. | 0.9 | 2 |
| 10077 | Host-Guest Complexes of [TriPip222], the Piperazine Analogue of [2.2.2]: Prediction of Ion Selectivity by Quantum Chemical Calculations VIII. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2016, 642, 395-402. | 0.6 | 9 |
| 10078 | Synthesis of Five-Porphyrin Nanorings by Using Ferrocene and Corannulene Templates. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 8358-8362. | 7.2 | 54 |
| 10079 | Analysis of a Compound Class with Triplet States Stabilized by Potentially Baird Aromatic [10]Annulenyl Dicationic Rings. <i>Chemistry - A European Journal</i> , 2016, 22, 2793-2800. | 1.7 | 30 |
| 10080 | Helical Oligoenes: Conformations, Bond Alternation, and Competing Through-Bond and Through-Space Transmission. <i>Chemistry - A European Journal</i> , 2016, 22, 4878-4888. | 1.7 | 21 |
| 10081 | Hückel's Rule of Aromaticity Categorizes Aromatic Boron Hydride Clusters. <i>Chemistry - A European Journal</i> , 2016, 22, 7437-7443. | 1.7 | 103 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10082 | Efficient Preparation of TMS CCl_2 Br and Its Use in Dichlorocyclopropanation of Electron-Deficient Alkenes. <i>Chemistry - A European Journal</i> , 2016, 22, 7609-7616. | 1.7 | 4 |
| 10083 | The catalytic effect of the $\langle \text{scp} \rangle \text{NH} \langle / \text{scp} \rangle \langle \text{sub} \rangle 3 \langle / \text{sub} \rangle$ base on the chemical events in the caryolene-forming carbocation cascade. <i>Journal of Computational Chemistry</i> , 2016, 37, 1068-1081. | 1.5 | 8 |
| 10084 | NIR-Raman spectrum and DFT calculations of okadaic acid DSP marine biotoxin microprobe. <i>Journal of Raman Spectroscopy</i> , 2016, 47, 636-642. | 1.2 | 7 |
| 10085 | Reaction between Azidyl Radicals and Alkynes: A Straightforward Approach to $\langle i \rangle \text{NH} \langle / i \rangle \hat{=} 1,2,3 \hat{=}$ Triazoles. <i>Chemistry - A European Journal</i> , 2016, 22, 911-915. | 1.7 | 33 |
| 10086 | The Valence States of Copernicium and Flerovium. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 2989-2992. | 1.0 | 10 |
| 10087 | Fluorescent Probes from Stable Aromatic Nitrile Oxides. <i>European Journal of Organic Chemistry</i> , 2016, 2016, 821-829. | 1.2 | 13 |
| 10088 | Synthesis and molecular properties of methoxy-substituted diindolo[3,2-b:2 $\hat{=}$ 2,3 $\hat{=}$ h]carbazoles for organic electronics obtained by a consecutive twofold Suzuki and twofold Cadogan reaction. <i>Journal of Materials Chemistry C</i> , 2016, 4, 6270-6279. | 2.7 | 37 |
| 10089 | Structure and magnetic properties of Saturn-shaped fullerene complexes with ferrocene and nickelocene dicarboxylic acids: DFT simulation. <i>Structural Chemistry</i> , 2016, 27, 281-284. | 1.0 | 3 |
| 10090 | Propionic acid derivatives confined in mesoporous silica: monomers or dimers? The case of ibuprofen investigated by static and dynamic ab initio simulations. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 6 |
| 10091 | Compressional behavior of MgCr 2O_4 spinel from first-principles simulation. <i>Science China Earth Sciences</i> , 2016, 59, 989-996. | 2.3 | 14 |
| 10092 | Electron Delocalization Range in Atoms and on Molecular Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3185-3194. | 2.3 | 11 |
| 10093 | General AMBER Force Field Parameters for Diphenyl Diselenides and Diphenyl Ditellurides. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4389-4400. | 1.1 | 22 |
| 10094 | Ethynyl substitution effect on the electronic excitation spectra of aniline. <i>Chemical Research in Chinese Universities</i> , 2016, 32, 268-271. | 1.3 | 0 |
| 10095 | Overview of band-edge and defect related luminescence in aluminum nitride. <i>Journal of Luminescence</i> , 2016, 178, 267-281. | 1.5 | 53 |
| 10096 | Theoretical study of optical activity of 1:1 hydrogen bond complexes of water with S-warfarin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 168, 180-189. | 2.0 | 4 |
| 10097 | Synthesis, structural characterization, antimicrobial activities and theoretical investigations of Part A: Molecular and Biomolecular Spectroscopy, 2016, 168, 190-198. | 2.0 | 8 |
| 10098 | Phase transition and dynamics of NH_3 ligands in $[\text{Zn}(\text{NH}_3)_4](\text{ReO}_4)_2$. <i>Vibrational Spectroscopy</i> , 2016, 86, 40-49. | 1.2 | 5 |
| 10099 | Metalloporphyrin-Nitroxyl Interactions: The Low-Energy States of Reduced Manganese, Iron, and Cobalt Porphyrin Nitrosyls. <i>Journal of Physical Chemistry B</i> , 2016, 120, 4972-4979. | 1.2 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10100 | Threshold ionization spectroscopic investigation of supersonic jet-cooled, laser-desorbed Tryptophan. <i>Chemical Physics Letters</i> , 2016, 657, 142-147. | 1.2 | 1 |
| 10101 | Deprotonation Induced Ligand Oxidation in a Ni ^{II} Complex of a Redox Noninnocent <i>N</i> -(2-Aminophenyl)benzene-1,2-diamine and Its Use in Catalytic Alcohol Oxidation. <i>Inorganic Chemistry</i> , 2016, 55, 6114-6123. | 1.9 | 47 |
| 10102 | Mitochondria-targeted aggregation induced emission theranostics: crucial importance of in situ activation. <i>Chemical Science</i> , 2016, 7, 6050-6059. | 3.7 | 83 |
| 10103 | Base pairing and structural insights into the 5-formylcytosine in RNA duplex. <i>Nucleic Acids Research</i> , 2016, 44, 4968-4977. | 6.5 | 25 |
| 10104 | Water exit pathways and proton pumping mechanism in B-type cytochrome c oxidase from molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2016, 1857, 1594-1606. | 0.5 | 15 |
| 10105 | Mechanistic Studies of Bismuth(V)-Mediated Thioglycoside Activation Reveal Differential Reactivity of Anomers. <i>Journal of Organic Chemistry</i> , 2016, 81, 5949-5962. | 1.7 | 19 |
| 10106 | Theoretical study of the hydrolysis mechanism of dihydrocoumarin catalyzed by serum paraoxonase 1 (PON1): different roles of Glu53 and His115 for catalysis. <i>RSC Advances</i> , 2016, 6, 60376-60384. | 1.7 | 2 |
| 10107 | Copper(I) Complexes of Pyridine-Bridged Phosphaalkene-Oxazoline Pincer Ligands. <i>Inorganic Chemistry</i> , 2016, 55, 6670-6678. | 1.9 | 24 |
| 10108 | Evidence of a Donor-Acceptor (Ir ^H) ⁺ SiR ₃ Interaction in a Trapped Ir(III) Silane Catalytic Intermediate. <i>Organometallics</i> , 2016, 35, 2207-2223. | 1.1 | 40 |
| 10109 | Structure and lattice dynamics of PrFe ₃ (BO ₃) ₄ : Ab initio calculation. <i>Physics of the Solid State</i> , 2016, 58, 1199-1206. | 0.2 | 0 |
| 10110 | Salicylic aldehyde and 2-N-tosylaminobenzaldehyde tetrazolyl hydrazones and their complexes. <i>Russian Journal of General Chemistry</i> , 2016, 86, 1064-1068. | 0.3 | 1 |
| 10111 | Optoelectronic properties of passivated and solvated (ZnO) 6 nanocluster - A DFT/TD-DFT study. <i>Materials Chemistry and Physics</i> , 2016, 181, 248-258. | 2.0 | 6 |
| 10112 | Molecular Dynamics Study of Nanoaggregation in Asphaltene Mixtures: Effects of the N, O, and S Heteroatoms. <i>Energy & Fuels</i> , 2016, 30, 5656-5664. | 2.5 | 73 |
| 10113 | Plasma-Enhanced Atomic Layer Deposition of SiN-AlN Composites for Ultra Low Wet Etch Rates in Hydrofluoric Acid. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 17599-17605. | 4.0 | 15 |
| 10114 | Interaction of amines with electrodes modified by polymeric complexes of Ni with salen-type ligands. <i>Electrochimica Acta</i> , 2016, 211, 726-734. | 2.6 | 15 |
| 10115 | High resolution X-ray and neutron diffraction studies on molecular complexes of chloranilic acid and lutidines. <i>CrystEngComm</i> , 2016, 18, 5697-5709. | 1.3 | 4 |
| 10116 | Density Functional Theory Calculation of pKa TM s of Thiols in Aqueous Solution Using Explicit Water Molecules and the Polarizable Continuum Model. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5726-5735. | 1.1 | 146 |
| 10117 | Enormous lattice distortion through an isomorphous phase transition in an organic-inorganic hybrid based on haloantimonate(_{iii}). <i>CrystEngComm</i> , 2016, 18, 6184-6194. | 1.3 | 22 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10118 | Electron transfer mechanism of catalytic superoxide dismutation via Cu(II) complexes: evidence of cupric superoxide/hydroperoxide species. Dalton Transactions, 2016, 45, 11898-11910. | 1.6 | 7 |
| 10119 | Rational design of new electrolyte materials for electrochemical double layer capacitors. Journal of Power Sources, 2016, 326, 541-548. | 4.0 | 61 |
| 10120 | Aplicyanins – brominated natural marine products with superbasic character. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2016, 71, 883-889. | 0.3 | 7 |
| 10121 | Bent and twisted: the electronic structure of 2-azapropenyl ions obtained by guanidine oxidation. RSC Advances, 2016, 6, 39323-39329. | 1.7 | 17 |
| 10122 | Absorption Band Shapes of a Push-Pull Dye Approaching the Cyanine Limit: A Challenging Case for First Principle Calculations. Journal of Physical Chemistry A, 2016, 120, 5581-5589. | 1.1 | 31 |
| 10123 | Proposed Modification of the Graphene Analogue Ni ₃ (HITP) ₂ To Yield a Semiconducting Material. Journal of Physical Chemistry C, 2016, 120, 15001-15008. | 1.5 | 67 |
| 10124 | Geometries, Binding Energies, Ionization Potentials, and Electron Affinities of Metal Clusters: Mg _n O _{±1} , $n = 1-7$. Journal of Physical Chemistry C, 2016, 120, 13275-13286. | 1.5 | 32 |
| 10125 | Tuning the electronic and photophysical properties of platinum(II) complexes through ancillary ligand modification: a theoretical study. Molecular Simulation, 2016, 42, 1035-1041. | 0.9 | 3 |
| 10126 | Adsorption of carbon monoxide on boroxol-ring-doped zigzag boron nitride nanotube: Electronic study via DFT. European Physical Journal Plus, 2016, 131, 1. | 1.2 | 6 |
| 10127 | Temperature-dependent fluorescence quenching of a cavitand derivative by copper ions. Chemical Physics Letters, 2016, 657, 60-64. | 1.2 | 1 |
| 10128 | Electrochemical Electron Transfer and Proton-Coupled Electron Transfer: Effects of Double Layer and Ionic Environment on Solvent Reorganization Energies. Journal of Chemical Theory and Computation, 2016, 12, 2917-2925. | 2.3 | 31 |
| 10129 | Impact of the Kohn-Sham Delocalization Error on the 4f Shell Localization and Population in Lanthanide Complexes. Journal of Chemical Theory and Computation, 2016, 12, 3109-3121. | 2.3 | 49 |
| 10130 | Surface-Enhanced Raman Scattering Due to Charge-Transfer Resonances: A Time-Dependent Density Functional Theory Study of Ag ₁₃ -4-Mercaptopyrindine. Journal of Physical Chemistry C, 2016, 120, 20721-20735. | 1.5 | 31 |
| 10131 | Electronic Structure of Low-Dimensional Carbon π -Systems. Journal of Physical Chemistry C, 2016, 120, 12362-12368. | 1.5 | 0 |
| 10132 | Factors Affecting the Production of Aromatic Immonium Ions in MALDI 157 nm Photodissociation Studies. Journal of the American Society for Mass Spectrometry, 2016, 27, 834-846. | 1.2 | 7 |
| 10133 | X-ray absorption spectroscopy of the chiral molecules fenchone, \pm -pinene, limonene and carvone in the C1s excitation region. Journal of Electron Spectroscopy and Related Phenomena, 2016, 207, 34-37. | 0.8 | 3 |
| 10134 | Influence of Iodide Intermolecular Interactions on Electronic Properties of Tin(IV) Iodide Semiconducting Complexes. Inorganic Chemistry, 2016, 55, 5935-5945. | 1.9 | 20 |
| 10135 | Near-Infrared Phosphorescent Iridium(III) Benzenorrole Complexes Possessing Pyridine-based Axial Ligands. Inorganic Chemistry, 2016, 55, 6223-6230. | 1.9 | 23 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10136 | Theoretical studies on oxidation-switchable second-order nonlinear optical responses of Metallo salen-Keggin polyoxometalate derivatives. <i>RSC Advances</i> , 2016, 6, 53438-53443. | 1.7 | 3 |
| 10137 | Surface complex of ZnTMPyP4 metalloporphyrin with double-stranded Poly(A)-Poly(U). <i>Journal of Inorganic Biochemistry</i> , 2016, 161, 83-90. | 1.5 | 12 |
| 10138 | Absolute configuration of the synthetic cannabinoid MDMB-CHMICA with its chemical characteristics in illegal products. <i>Forensic Toxicology</i> , 2016, 34, 344-352. | 1.4 | 18 |
| 10139 | Properties of two-dimensional insulators: A DFT study of bimetallic oxide CrW ₂ O ₉ clusters adsorption on MgO ultrathin films. <i>Applied Surface Science</i> , 2016, 379, 213-222. | 3.1 | 5 |
| 10140 | How half sandwich ruthenium compounds interact with DNA while not being hydrolyzed; a comparative study. <i>Journal of Inorganic Biochemistry</i> , 2016, 160, 12-23. | 1.5 | 9 |
| 10141 | Jahn-Teller distortion in tris[4,4,4-trifluoro-1-(2-thienyl)-1,3-butanedionato]manganese(III) isomers: An X-ray and computational study. <i>Journal of Molecular Structure</i> , 2016, 1119, 48-53. | 1.8 | 11 |
| 10142 | Adsorption properties of boroxol ring doped zigzag boron nitride nanotube toward NO molecule using DFT. <i>International Journal of Modern Physics B</i> , 2016, 30, 1650101. | 1.0 | 1 |
| 10143 | Chloromethyl-oxirane and chloromethyl-thiirane in liquid phase: A joint experimental and quantum chemical study. <i>Chemical Physics</i> , 2016, 473, 24-31. | 0.9 | 8 |
| 10144 | Sulfur and carbon as heteroatoms in ferrathiocarboranes. <i>Polyhedron</i> , 2016, 113, 109-114. | 1.0 | 0 |
| 10145 | Force dependence of the infrared spectra of polypropylene calculated with density functional theory. <i>Polymer Degradation and Stability</i> , 2016, 128, 294-299. | 2.7 | 9 |
| 10146 | The Relativistic Effects on the Carbon-Carbon Coupling Constants Mediated by a Heavy Atom. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5624-5634. | 1.1 | 10 |
| 10147 | New Insights into Mechanism of Molybdenum(VI)-Dioxo Complex Catalyzed Hydrosilylation of Carbonyls: An Alternative Model for Activating Si-H Bond. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4167-4178. | 1.1 | 6 |
| 10148 | Anthrax Edema Factor: An Ion-Adaptive Mechanism of Catalysis with Increased Transition-State Conformational Flexibility. <i>Journal of Physical Chemistry B</i> , 2016, 120, 6504-6514. | 1.2 | 7 |
| 10149 | Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulations Reveal a Rotationally Fluid Adsorption State of β -Pinene on Silica. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12578-12589. | 1.5 | 29 |
| 10150 | Surface-Induced Anisotropic Binding of a Rhenium CO ₂ -Reduction Catalyst on Rutile TiO ₂ (110) Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 20970-20977. | 1.5 | 44 |
| 10151 | Theoretical Studies on the Mechanism of Thioesterase-Catalyzed Macrocyclization in Erythromycin Biosynthesis. <i>ACS Catalysis</i> , 2016, 6, 4369-4378. | 5.5 | 32 |
| 10152 | Lactobacillus plantarum WCFS1 β -Fructosidase: Evidence for an Open Funnel-Like Channel Through the Catalytic Domain with Importance for the Substrate Selectivity. <i>Applied Biochemistry and Biotechnology</i> , 2016, 180, 1056-1075. | 1.4 | 3 |
| 10153 | Spirooxazine-Fulgide Biphotochromic Molecular Switches with Nonlinear Optical Responses across Four States. <i>Journal of Physical Chemistry C</i> , 2016, 120, 14840-14853. | 1.5 | 37 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10154 | Synthesis, characterization, single crystal X-ray structure, EPR and theoretical studies of a new hybrid inorganic-organic compound [Cu(Hdien) ₂ (H ₂ O) ₂](pnb) ₄ ·4H ₂ O and its structural comparison with related [Cu(en) ₂ (H ₂ O) ₂](pnb) ₂ . <i>Journal of Molecular Structure</i> , 2016, 1123, 124-132. | 1.8 | 16 |
| 10155 | The influence of the DFT approach on the structure and relative stability of models for cellulose I allomorphs. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 7 |
| 10156 | Structure and Frontier Molecular Orbital (FMO) energies of \pm -Keggin-type polyoxometalate [PW ₁₂ O ₄₀] ³⁻ : A systematical study with different functionals of density functional theory. <i>Computational and Theoretical Chemistry</i> , 2016, 1089, 28-34. | 1.1 | 9 |
| 10157 | Metal-organic frameworks in cadmium(II) complexes with 5-methoxyindole-2-carboxylic acid: structure, vibrational spectra and DFT calculations. <i>Journal of Molecular Structure</i> , 2016, 1123, 14-23. | 1.8 | 12 |
| 10158 | Bis-Tridentate Iridium(III) Phosphors Bearing Functional 2-Phenyl-6-(imidazol-2-ylidene)pyridine and 2-(Pyrazol-3-yl)-6-phenylpyridine Chelates for Efficient OLEDs. <i>Organometallics</i> , 2016, 35, 1813-1824. | 1.1 | 63 |
| 10159 | Structural and spectroscopic characterization of two new blue luminescent pyridylbenzimidazole zinc(II) complexes. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2016, 72, 491-497. | 0.2 | 7 |
| 10160 | Iridium(III) 2-Phenylbenzimidazole Complexes: Synthesis, Structure, Optical Properties, and Applications in Dye-Sensitized Solar Cells. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 347-354. | 1.0 | 36 |
| 10161 | Saturn Systems. <i>Journal of Computational Chemistry</i> , 2016, 37, 194-209. | 1.5 | 20 |
| 10162 | Improving $\langle B \rangle$ heats of formation with three-dimensional molecular descriptors. <i>Journal of Computational Chemistry</i> , 2016, 37, 1175-1190. | 1.5 | 11 |
| 10163 | Multipole moments for embedding potentials: Exploring different atomic allocation algorithms. <i>Journal of Computational Chemistry</i> , 2016, 37, 1887-1896. | 1.5 | 6 |
| 10164 | Syntheses, structures and properties of four metal-organic frameworks from chlorophenyl imidazole dicarboxylates. <i>Journal of Coordination Chemistry</i> , 2016, 69, 2231-2246. | 0.8 | 5 |
| 10165 | EPR study of gamma-irradiated 2-Bromo-4-methoxyacetophenone single crystals. <i>Radiation Effects and Defects in Solids</i> , 2016, 171, 214-222. | 0.4 | 3 |
| 10166 | Mechanism and Site Selectivity in Visible-Light Photocatalyzed C-H Functionalization: Insights from DFT Calculations. <i>Journal of Organic Chemistry</i> , 2016, 81, 7110-7120. | 1.7 | 14 |
| 10167 | Description of the Charge Transfer States at the Pentacene/C ₆₀ Interface: Combining Range-Separated Hybrid Functionals with the Polarizable Continuum Model. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2616-2621. | 2.1 | 66 |
| 10168 | Computational and experimental investigations of one-step conversion of poly(carbonate)s into value-added poly(aryl ether sulfone)s. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 7722-7726. | 3.3 | 62 |
| 10169 | Vibrational Signatures of Conformer-Specific Intramolecular Interactions in Protonated Tryptophan. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5598-5608. | 1.1 | 32 |
| 10170 | Tetracarbalane structures: nido polyhedra and non-spherical deltahedra. <i>Dalton Transactions</i> , 2016, 45, 11528-11539. | 1.6 | 5 |
| 10171 | Introducing DDEC6 atomic population analysis: part 2. Computed results for a wide range of periodic and nonperiodic materials. <i>RSC Advances</i> , 2016, 6, 45727-45747. | 1.7 | 351 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 10172 | NMR properties of hydrogen-bonded glycine cluster in gas phase. <i>Journal of Molecular Structure</i> , 2016, 1123, 55-65. | 1.8 | 6 |
| 10173 | The adsorption of rifampicin on gold or silver surfaces mediated by 2-mercaptoethanol investigated by surface-enhanced Raman scattering spectroscopy. <i>Vibrational Spectroscopy</i> , 2016, 86, 75-80. | 1.2 | 12 |
| 10174 | Passivation of Molecular n-doping: Exploring the Limits of Air Stability. <i>Advanced Functional Materials</i> , 2016, 26, 3730-3737. | 7.8 | 46 |
| 10175 | Phosphorescent Nanocluster Light-Emitting Diodes. <i>Advanced Materials</i> , 2016, 28, 320-326. | 11.1 | 67 |
| 10176 | Highly Active Titanocene Catalysts for Epoxide Hydrosilylation: Synthesis, Theory, Kinetics, EPR Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 7671-7675. | 7.2 | 57 |
| 10177 | Computational Insight on CO ₂ Fixation to Produce Styrene Carbonate Assisted by a Single-Center Aluminum(III) Catalyst and Quaternary Ammonium Salts. <i>ChemCatChem</i> , 2016, 8, 1167-1175. | 1.8 | 28 |
| 10178 | Highly Convergent Synthesis of Intensively Blue Emissive Furo[2,3- <i>c</i>]isoquinolines by a Palladium-Catalyzed Cyclization Cascade of Unsaturated Ugi Products. <i>Chemistry - A European Journal</i> , 2016, 22, 2020-2031. | 1.7 | 30 |
| 10179 | Structures and Chemical Bonding in NbS _n (n=3,4,5) Clusters: Effects of Sulfur Content and Charge States. <i>Journal of Cluster Science</i> , 2016, 27, 387-401. | 1.7 | 3 |
| 10180 | Thermodynamic properties of indan: Experimental and computational results. <i>Journal of Chemical Thermodynamics</i> , 2016, 96, 41-51. | 1.0 | 10 |
| 10181 | Oligothiophene wires: impact of torsional conformation on the electronic structure. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4842-4849. | 1.3 | 11 |
| 10182 | Problems, successes and challenges for the application of dispersion-corrected density-functional theory combined with dispersion-based implicit solvent models to large-scale hydrophobic self-assembly and polymorphism. <i>Molecular Simulation</i> , 2016, 42, 494-510. | 0.9 | 13 |
| 10183 | Homogeneous Photocatalytic Water Oxidation with a Dinuclear Co ^{III} -Pyridylmethylamine Complex. <i>Inorganic Chemistry</i> , 2016, 55, 1154-1164. | 1.9 | 73 |
| 10184 | Density Functional Study of Nickel-N-Heterocyclic Carbene Catalyzed C=O Bond Hydrogenolysis of Methyl Phenyl Ether: The Concerted β -H Transfer Mechanism. <i>ACS Catalysis</i> , 2016, 6, 1477-1486. | 5.5 | 32 |
| 10185 | A New Method for Describing the Mechanism of a Chemical Reaction Based on the Unified Reaction Valley Approach. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 650-663. | 2.3 | 41 |
| 10186 | Oxidative Cleavage of the β -O-4 Linkage of Lignin by Transition Metals: Catalytic Properties and the Performance of Density Functionals. <i>Journal of Physical Chemistry A</i> , 2016, 120, 737-746. | 1.1 | 25 |
| 10187 | DNA binding properties, histidine interaction and cytotoxicity studies of water soluble ruthenium(II) terpyridine complexes. <i>Dalton Transactions</i> , 2016, 45, 4633-4646. | 1.6 | 70 |
| 10188 | Asymmetric Michael Additions of 4-Hydroxycoumarin to β -Nitrostyrenes with Chiral, Bifunctional Hydrogen-Bonding Catalysts. <i>Journal of Organic Chemistry</i> , 2016, 81, 1762-1768. | 1.7 | 22 |
| 10189 | Rh ₂ (II,III) Catalysts with Chelating Carboxylate and Carboxamidate Supports: Electronic Structure and Nitrene Transfer Reactivity. <i>Journal of the American Chemical Society</i> , 2016, 138, 2327-2341. | 6.6 | 95 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10190 | A theoretical study on charge transport of dithiolene nickel complexes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 6259-6267. | 1.3 | 7 |
| 10191 | Origin of Electrochemical, Structural, and Transport Properties in Nonaqueous Zinc Electrolytes. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 3021-3031. | 4.0 | 181 |
| 10192 | Type-I dyotropic rearrangement for 1,2-disubstituted cyclohexanes: substitution effect on activation energy. <i>RSC Advances</i> , 2016, 6, 10549-10556. | 1.7 | 6 |
| 10193 | Gradient-regulated connection-based correction for the PBE exchange: the PBEtrans model. <i>Molecular Physics</i> , 2016, 114, 1059-1065. | 0.8 | 3 |
| 10194 | Ionic Liquids as Electrolytes for Electrochemical Double-Layer Capacitors: Structures that Optimize Specific Energy. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 3396-3406. | 4.0 | 175 |
| 10195 | Development of a ReaxFF reactive force field for Si/Ge/H systems and application to atomic hydrogen bombardment of Si, Ge, and SiGe (100) surfaces. <i>Surface Science</i> , 2016, 646, 253-260. | 0.8 | 33 |
| 10196 | A salification-induced charge transfer effect for improving the resistive memory performance of azo derivative-based devices. <i>RSC Advances</i> , 2016, 6, 10471-10477. | 1.7 | 6 |
| 10197 | Benzimidazole-thiazole based NLOphoric styryl dyes with solid state emission " Synthesis, photophysical, hyperpolarizability and TD-DFT studies. <i>Dyes and Pigments</i> , 2016, 128, 111-123. | 2.0 | 36 |
| 10198 | A fluorescent coumarin-thiophene hybrid as a ratiometric chemosensor for anions: Synthesis, photophysics, anion sensing and orbital interactions. <i>Journal of Molecular Structure</i> , 2016, 1108, 269-277. | 1.8 | 34 |
| 10199 | Pyrazole based NLOphores: Synthesis, photophysical, DFT, TDDFT studies. <i>Dyes and Pigments</i> , 2016, 127, 116-127. | 2.0 | 30 |
| 10200 | Reaction mechanisms of the Rh-catalyzed dehydrogenative aryl-aryl bond formation reaction of tertiary benzamide with bromobenzene: A theoretical study. <i>Journal of Organometallic Chemistry</i> , 2016, 803, 1-8. | 0.8 | 2 |
| 10201 | Investigation of bromine atom transfer mechanism from an alkyl bromide molecule to an O-bonded alkyl group in a FAU zeolite by the ONIOM method. <i>Microporous and Mesoporous Materials</i> , 2016, 226, 1-9. | 2.2 | 10 |
| 10202 | Calculations of Solvation Free Energy through Energy Reweighting from Molecular Mechanics to Quantum Mechanics. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 499-511. | 2.3 | 78 |
| 10203 | Tuning nitrogen species to control the charge carrier concentration in highly doped graphene. <i>2D Materials</i> , 2016, 3, 011001. | 2.0 | 27 |
| 10204 | Carbon monoxide protonation in condensed phases and bonding to surface superacidic Brønsted centers. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4871-4880. | 1.3 | 16 |
| 10205 | Mechanism and enantioselectivity in α -alkylation of carbonyl compounds via photoredox organocatalysis: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2016, 1078, 113-122. | 1.1 | 5 |
| 10206 | Synthesis and structure of novel triphenylarsine-substituted tungsten(0) Fischer carbene complexes. <i>Journal of Molecular Structure</i> , 2016, 1105, 205-213. | 1.8 | 6 |
| 10207 | Br ₂ as a novel Lewis acid catalyst for Friedel-Crafts alkylation of indoles with α,β -unsaturated ketones. <i>Tetrahedron Letters</i> , 2016, 57, 1027-1030. | 0.7 | 22 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10208 | From C ₆₀ to Infinity: Large-Scale Quantum Chemistry Calculations of the Heats of Formation of Higher Fullerenes. <i>Journal of the American Chemical Society</i> , 2016, 138, 1420-1429. | 6.6 | 32 |
| 10209 | High-efficiency and low efficiency roll-off near-infrared fluorescent OLEDs through triplet fusion. <i>Chemical Science</i> , 2016, 7, 2888-2895. | 3.7 | 88 |
| 10210 | Ab initio investigation of majorite and pyrope garnets: Lattice dynamics and vibrational spectra. <i>American Mineralogist</i> , 2016, 101, 162-174. | 0.9 | 14 |
| 10211 | Extraordinary Mechanism of the Diels-Alder Reaction: Investigation of Stereochemistry, Charge Transfer, Charge Polarization, and Biradicaloid Formation. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1097-1111. | 1.1 | 37 |
| 10212 | Novel NLOphoric 2-methoxy carbazole-based push pull chromophores: Synthesis, photophysical properties and TD-DFT Study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 321, 63-71. | 2.0 | 23 |
| 10213 | Structure, NMR and Electronic Spectra of [<i>m.n.n</i>]Paracyclophanes with Varying Bridges Lengths (<i>m, n = 2-4</i>). <i>Journal of Physical Chemistry A</i> , 2016, 120, 724-736. | 1.1 | 10 |
| 10214 | Anodic Methods for Covalent Attachment of Ethynylferrocenes to Electrode Surfaces: Comparison of Ethynyl Activation Processes. <i>Langmuir</i> , 2016, 32, 1645-1657. | 1.6 | 14 |
| 10215 | Multi-level molecular modelling for plasma medicine. <i>Journal Physics D: Applied Physics</i> , 2016, 49, 054002. | 1.3 | 26 |
| 10216 | Preparation of Ru^{I} - and Ru^{II} -isomers of mono-Ru-substituted Dawson-type phosphotungstates with an aqua ligand and comparison of their redox potentials, catalytic activities, and thermal stabilities with Keggin-type derivatives. <i>Dalton Transactions</i> , 2016, 45, 3715-3726. | 1.6 | 16 |
| 10217 | Exploring excited state properties of 7-hydroxy and 7-methoxy 4-methylcoumarin: a combined time-dependent density functional theory/effective fragment potential study. <i>New Journal of Chemistry</i> , 2016, 40, 2211-2219. | 1.4 | 4 |
| 10218 | What can tell the quantum chemical topology on carbon-astatine bonds?. <i>Molecular Physics</i> , 2016, 114, 1326-1333. | 0.8 | 11 |
| 10219 | Computational and DNMR Analysis of the Conformational Isomers and Stereodynamics of Secondary 2,2-Bis(aryl)-Bis(amide)s. <i>Journal of Organic Chemistry</i> , 2016, 81, 89-99. | 1.7 | 6 |
| 10220 | Solving the Pericyclic-Pseudopericyclic Puzzle in the Ring-Closure Reactions of 1,2,4,6-Heptatetraene Derivatives. <i>Journal of Organic Chemistry</i> , 2016, 81, 404-414. | 1.7 | 29 |
| 10221 | Octahedral aromaticity in X_6 clusters ($\text{X} = \text{C, Si, Ge, Sn, Pb, Bi, Sb, As, N, P, As, Se, Te, Po, S, Se, Te, Po, S, Se, Te, Po}$) | 1.3 | 12 |
| 10222 | Global optimization of clusters of rigid molecules using the artificial bee colony algorithm. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3003-3010. | 1.3 | 292 |
| 10223 | Preferred Geometries and Energies of Sulfur-Sulfur Interactions in Crystal Structures. <i>Crystal Growth and Design</i> , 2016, 16, 632-639. | 1.4 | 54 |
| 10224 | Quantifying Electron Delocalization in Electrides. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 79-91. | 2.3 | 15 |
| 10225 | A DFT Study on Rh-Catalyzed Asymmetric Dearomatization of 2-Naphthols Initiated with H ₂ O ₂ Activation: A Refined Reaction Mechanism and Origins of Multiple Selectivity. <i>ACS Catalysis</i> , 2016, 6, 262-271. | 5.5 | 63 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 10226 | Synthesis and optoelectronic properties of chemically modified bi-fluorenylidenes. <i>Journal of Materials Chemistry C</i> , 2016, 4, 3798-3808. | 2.7 | 15 |
| 10227 | Cytisine basicity, solvation, log P, and log D theoretical determination as tool for bioavailability prediction. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 63, 15-21. | 1.3 | 20 |
| 10228 | Induction of Cytotoxicity in Pyridine Analogues of the Anti-metastatic Ru(III) Complex NAMI-A by Ferrocene Functionalization. <i>Inorganic Chemistry</i> , 2016, 55, 177-190. | 1.9 | 31 |
| 10229 | New metabolites from the alga-derived fungi <i>Penicillium thomii</i> Maire and <i>Penicillium lividum</i> Westling. <i>Phytochemistry Letters</i> , 2016, 15, 7-12. | 0.6 | 19 |
| 10230 | Electronically Excited States of Higher Acenes up to Nonacene: A Density Functional Theory/Multireference Configuration Interaction Study. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 305-312. | 2.3 | 43 |
| 10231 | Performance of some DFT functionals with dispersion on modeling of the translational isomers of a solvent-switchable [2]rotaxane. <i>Journal of Molecular Structure</i> , 2016, 1107, 31-38. | 1.8 | 13 |
| 10232 | Benzoindolium-triarylborane conjugates: a ratiometric fluorescent chemodosimeter for the detection of cyanide ions in aqueous medium. <i>Dalton Transactions</i> , 2016, 45, 5014-5020. | 1.6 | 34 |
| 10233 | A reversible fluorescence probe for detection of ClO ⁻ /AA redox cycle in aqueous solution and in living cells. <i>Talanta</i> , 2016, 147, 468-472. | 2.9 | 46 |
| 10234 | Raman, infrared and DFT studies of N ² -(adamantan-2-ylidene)benzohydrazide, a potential antibacterial agent. <i>Journal of Molecular Structure</i> , 2016, 1115, 258-266. | 1.8 | 22 |
| 10235 | Exact exchange and the density functional theory of metal-to-ligand charge-transfer in fac-Ir(ppy) ₃ . <i>Organic Electronics</i> , 2016, 33, 110-115. | 1.4 | 11 |
| 10236 | Material Exhibiting Efficient CO ₂ Adsorption at Room Temperature for Concentrations Lower Than 1000 ppm: Elucidation of the State of Barium Ion Exchanged in an MFI-Type Zeolite. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 8821-8833. | 4.0 | 15 |
| 10237 | Properties and reactivity of nucleic acids relevant to epigenomics, transcriptomics, and therapeutics. <i>Chemical Society Reviews</i> , 2016, 45, 2637-2655. | 18.7 | 34 |
| 10238 | A combined computational and experimental investigation of the oxidative ring-opening of cyclic ethers by oxoammonium cations. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 3883-3888. | 1.5 | 16 |
| 10239 | Novel 2H-pyran-3-carbonitrile dyes – Synthesis, solvatochromism study, and DFT, TD-DFT computations. <i>Journal of Luminescence</i> , 2016, 176, 298-308. | 1.5 | 7 |
| 10240 | Tautomerism in N-(2-hydroxy-1-naphthylidene)amino acids and the search for an answer to the difficult question about where the proton belongs. <i>Journal of Molecular Structure</i> , 2016, 1117, 37-48. | 1.8 | 7 |
| 10241 | Spin-State Energetics of Fe(III) and Ru(III) Aqua Complexes: Accurate ab Initio Calculations and Evidence for Huge Solvation Effects. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1592-1605. | 2.3 | 38 |
| 10242 | On the molecular basis of the activity of the antimalarial drug chloroquine: EXAFS-assisted DFT evidence of a direct Fe-N bond with free heme in solution. <i>Physica Scripta</i> , 2016, 91, 023001. | 1.2 | 7 |
| 10243 | Photoluminescence of a New Material: Cyclometalated C ⁺ Thiazole-2-ylidene Platinum(II) Complexes. <i>Organometallics</i> , 2016, 35, 959-971. | 1.1 | 34 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10244 | Formation of a robust Ru ₄ O ₄ skeleton with two Ru ₂ (CO) ₄ units in crissâ€‘cross configuration. RSC Advances, 2016, 6, 31196-31201. | 1.7 | 3 |
| 10245 | Indole-containing new types of dyes and their UVâ€‘vis and NMR spectra and electronic structures: Experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 162, 61-68. | 2.0 | 10 |
| 10246 | Coumarin Push-Pull NLOphores with Red Emission: Solvatochromic and Theoretical Approach. Journal of Fluorescence, 2016, 26, 949-962. | 1.3 | 32 |
| 10247 | Geometrical isomers of tris(Î²-diketonato)metal(III) complexes for M = Cr or Co: Synthesis, X-ray structures and DFT study. Inorganica Chimica Acta, 2016, 447, 59-65. | 1.2 | 11 |
| 10248 | Investigation into 9(S)-HPODE-derived allene oxide to cyclopentenone cyclization mechanism via diradical oxyallyl intermediates. Organic and Biomolecular Chemistry, 2016, 14, 3544-3557. | 1.5 | 10 |
| 10249 | Studies on the mechanism of quaternization of the catharanthine part of vinblastine and vincristine. Tetrahedron Letters, 2016, 57, 1672-1677. | 0.7 | 3 |
| 10250 | Expanding DP4: application to drug compounds and automation. Organic and Biomolecular Chemistry, 2016, 14, 3943-3949. | 1.5 | 40 |
| 10251 | Mechanistic insight into the selective cyclization of aryl nitrones to indolines via Rh(<i>iii</i>) catalyst: a theoretical study. RSC Advances, 2016, 6, 23265-23271. | 1.7 | 10 |
| 10252 | Tuning Side Arm Electronics in Unsymmetrical Cyclootriazadisulfonamide (CADA) Endoplasmic Reticulum (ER) Translocation Inhibitors to Improve their Human Cluster of Differentiation 4 (CD4) Receptor Down-Modulating Potencies. Journal of Medicinal Chemistry, 2016, 59, 2633-2647. | 2.9 | 16 |
| 10253 | Molybdatricarbaboranes as examples of isocloso metallaborane deltahedra with three carbon vertices. Journal of Computational Chemistry, 2016, 37, 64-69. | 1.5 | 1 |
| 10254 | Rotational Isomerism, Electronic Structures, and Basicity Properties of â€‘Fully-Reducedâ€™ V ₁₄ -type Heteropolyoxovanadates. Inorganic Chemistry, 2016, 55, 3777-3788. | 1.9 | 18 |
| 10255 | Heats of formation of platonic hydrocarbon cages by means of highâ€‘level thermochemical procedures. Journal of Computational Chemistry, 2016, 37, 49-58. | 1.5 | 66 |
| 10256 | Reâ€‘evaluation of the bond lengthâ€‘bond strength rule: The stronger bond is not always the shorter bond. Journal of Computational Chemistry, 2016, 37, 130-142. | 1.5 | 88 |
| 10257 | Spectroscopic and QM/MM investigations of Chloroperoxidase catalyzed degradation of orange G. Archives of Biochemistry and Biophysics, 2016, 596, 1-9. | 1.4 | 10 |
| 10258 | Structural and magnetic properties of heptacoordinated Mn ^{II} complexes containing a 15-membered pyridine-based macrocycle and halido/pseudohalido axial coligands. RSC Advances, 2016, 6, 34674-34684. | 1.7 | 17 |
| 10259 | GROMOS polarisable model for acetone. Molecular Physics, 2016, 114, 845-854. | 0.8 | 7 |
| 10260 | Experimental and Theoretical Investigation of a Series of Novel Dimanganese(III) 1/4-Hydroxo Bisporphyrins: Magnetoâ€‘Structural Correlation and Effect of Metal Spin on Porphyrin Core Deformation. Inorganic Chemistry, 2016, 55, 3239-3251. | 1.9 | 28 |
| 10261 | Automated Selection of Active Orbital Spaces. Journal of Chemical Theory and Computation, 2016, 12, 1760-1771. | 2.3 | 237 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10262 | Thermostable Artificial Solid-Electrolyte Interface Layer Covalently Linked to Graphite for Lithium Ion Battery: Molecular Dynamics Simulations. <i>Journal of the Electrochemical Society</i> , 2016, 163, A917-A922. | 1.3 | 16 |
| 10263 | Exploring the limits of recent exchangeâ€‘correlation functionals in modeling lithium/benzene interaction. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 26 |
| 10264 | Effect of cis / trans isomerism on selective oxidation of olefins with nitrous oxide. <i>Tetrahedron</i> , 2016, 72, 2501-2506. | 1.0 | 7 |
| 10265 | Four-Component Damped Density Functional Response Theory Study of UV/Vis Absorption Spectra and Phosphorescence Parameters of Group 12 Metal-Substituted Porphyrins. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2324-2334. | 2.3 | 9 |
| 10266 | Assessment of DFT for Computing Sum Frequency Generation Spectra of an Epoxydiol and a Deuterated Isotopologue at Fused Silica/Vapor Interfaces. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1919-1927. | 1.2 | 17 |
| 10267 | Fourth stable radical species in X-irradiated solid-state sucrose. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 10983-10991. | 1.3 | 5 |
| 10268 | Mechanistic Study of Cellulose Hydrolysis by Carbon Catalysts. <i>Springer Theses</i> , 2016, , 77-112. | 0.0 | 2 |
| 10269 | Electron Detachment and Subsequent Structural Changes of Water Clusters. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1065-1073. | 1.1 | 5 |
| 10270 | Heterointerface Screening Effects between Organic Monolayers and Monolayer Transition Metal Dichalcogenides. <i>ACS Nano</i> , 2016, 10, 2476-2484. | 7.3 | 87 |
| 10271 | Modelling metal centres, acid sites and reaction mechanisms in microporous catalysts. <i>Faraday Discussions</i> , 2016, 188, 235-255. | 1.6 | 29 |
| 10272 | Aurophilicity in Action: Fine-Tuning the Gold(I)â€‘Gold(I) Distance in the Excited State To Modulate the Emission in a Series of Dinuclear Homoleptic Gold(I)â€‘NHC Complexes. <i>Inorganic Chemistry</i> , 2016, 55, 4720-4732. | 1.9 | 59 |
| 10273 | Polymorphism and conformerism in chalcones. <i>CrystEngComm</i> , 2016, 18, 2144-2154. | 1.3 | 13 |
| 10274 | Multi-conformer molecules in solutions: an NMR-based DFT/MP2 conformational study of two glucopyranosides of a vitamin E model compound. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 3142-3158. | 1.5 | 17 |
| 10275 | Assignment of absolute stereostructures through quantum mechanics electronic and vibrational circular dichroism calculations. <i>Journal of Asian Natural Products Research</i> , 2016, 18, 72-91. | 0.7 | 6 |
| 10276 | First Principle Analysis of (10-Boranyl anthracene-9-yl)borane-Based Molecular Single-Electron Transistor for High-Speed Low-Power Electronics. <i>IEEE Transactions on Electron Devices</i> , 2016, 63, 1232-1238. | 1.6 | 14 |
| 10277 | Enantiospecific formation of a metal-mediated base pair inside a DNA duplex. <i>Inorganica Chimica Acta</i> , 2016, 452, 181-187. | 1.2 | 28 |
| 10278 | Comparative study of H ₂ adsorption on B ₂₄ N ₂₄ , Al ₂₄ N ₂₄ and B ₁₂ Al ₁₂ N ₂₄ clusters. <i>Computational Materials Science</i> , 2016, 117, 71-75. | 1.4 | 21 |
| 10279 | Binuclear bromide complex of Bi(III): Thermally induced changes in optical properties. <i>Journal of Molecular Structure</i> , 2016, 1112, 21-24. | 1.8 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10280 | Deactivation pathways of thiophene and oligothiophenes: internal conversion versus intersystem crossing. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7903-7915. | 1.3 | 38 |
| 10281 | The stereoselectivities of tributyltin hydride-mediated reductions of 5-bromo- α -glucuronides to α -iduronides are dependent on the anomeric substituent: syntheses and DFT calculations. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 2950-2960. | 1.5 | 12 |
| 10282 | Ionisation and (de-)protonation energies of gas-phase amino acids from an optimally tuned range-separated hybrid functional. <i>Molecular Physics</i> , 2016, 114, 1218-1224. | 0.8 | 11 |
| 10283 | Synthesis of Main-Chain Poly(fullerene)s from a Sterically Controlled Azomethine Ylide Cycloaddition Polymerization. <i>Macromolecules</i> , 2016, 49, 1681-1691. | 2.2 | 20 |
| 10284 | A screened automated structural search with semiempirical methods. <i>Chemical Physics Letters</i> , 2016, 648, 119-123. | 1.2 | 5 |
| 10285 | Synthesis of β -extended N-fused heteroacenes via regioselective Cadogan reaction. <i>Tetrahedron Letters</i> , 2016, 57, 1468-1472. | 0.7 | 8 |
| 10286 | Mechanisms and origins of the switchable regioselectivity of FeBr_3 -catalyzed [1,2]-aryl and [1,2]-alkyl shifts of α -aryl aldehydes. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 2522-2536. | 1.5 | 10 |
| 10287 | Visualisation of charge-transfer excitations in donor-acceptor molecules using the particle-hole map: a case study. <i>Molecular Physics</i> , 2016, 114, 1365-1373. | 0.8 | 6 |
| 10288 | One- and two-photon activity of diketopyrrolopyrrole-Zn-porphyrin conjugates: linear and quadratic density functional response theory applied to model systems. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 4 |
| 10289 | Gauging the Performance of Density Functionals for Lanthanide-Containing Molecules. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1259-1266. | 2.3 | 39 |
| 10290 | Mixed-Valence Cations of Di(carbazol-9-yl) Biphenyl, Tetrahydropyrene, and Pyrene Derivatives. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3156-3166. | 1.5 | 19 |
| 10291 | Gauge effects in local hybrid functionals evaluated for weak interactions and the GMTKN30 test set. <i>Molecular Physics</i> , 2016, 114, 1118-1127. | 0.8 | 26 |
| 10292 | Proton Mobility in b^2 Ion Formation and Fragmentation Reactions of Histidine-Containing Peptides. <i>Journal of the American Society for Mass Spectrometry</i> , 2016, 27, 487-497. | 1.2 | 18 |
| 10293 | Unexpected Scholl Reaction of 6,7,13,14-Tetraarylbenzo[<i>k</i>]tetraphene: Selective Formation of Five-Membered Rings in Polycyclic Aromatic Hydrocarbons. <i>Journal of the American Chemical Society</i> , 2016, 138, 2602-2608. | 6.6 | 103 |
| 10294 | Mechanistic investigation of palladium-catalyzed amidation of aryl halides. <i>Journal of Molecular Modeling</i> , 2016, 22, 53. | 0.8 | 6 |
| 10295 | Transferability of different classical force fields for right and left handed α -helices constructed from enantiomeric amino acids. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5550-5563. | 1.3 | 5 |
| 10296 | Highly selective and sensitive fluorescence detection of Zn^{2+} and Cd^{2+} ions by using an acridine sensor. <i>Dalton Transactions</i> , 2016, 45, 5689-5699. | 1.6 | 24 |
| 10297 | Strong Field Molecular Ionization in the Impulsive Limit: Freezing Vibrations with Short Pulses. <i>Physical Review Letters</i> , 2016, 116, 063002. | 2.9 | 32 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10298 | Diamond and its olivine inclusions: A strange relation revealed by ab initio simulations. <i>Earth and Planetary Science Letters</i> , 2016, 435, 31-35. | 1.8 | 20 |
| 10299 | Direct Observation of Early-Stage Quantum Dot Growth Mechanisms with High-Temperature Ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2016, 120, 2472-2483. | 1.5 | 20 |
| 10300 | Raman and DFT study of methimazole chemisorbed on gold colloidal nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5974-5980. | 1.3 | 31 |
| 10301 | Extension of the interacting quantum atoms (IQA) approach to B3LYP level density functional theory (DFT). <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20986-21000. | 1.3 | 140 |
| 10302 | How well can B3LYP heats of formation be improved by dispersion correction models?. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 7 |
| 10303 | Spectroscopic Evidence for a $3d^{10}$ Ground State Electronic Configuration and Ligand Field Inversion in $[\text{Cu}(\text{CF}_3)_3]^{+}$. <i>Journal of the American Chemical Society</i> , 2016, 138, 1922-1931. | 6.6 | 99 |
| 10304 | A Study on Catalytic Conversion of Non-Food Biomass into Chemicals. Springer Theses, 2016, , . | 0.0 | 5 |
| 10305 | Development of an exchange-correlation functional with uncertainty quantification capabilities for density functional theory. <i>Journal of Computational Physics</i> , 2016, 311, 173-195. | 1.9 | 29 |
| 10306 | A mechanism for the hole-mediated water photooxidation on $\text{TiO}_2(110)$ surfaces. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 074002. | 0.7 | 23 |
| 10307 | Radical Monocationic Guanidino-Functionalized Aromatic Compounds (GFAs) as Bridging Ligands in Dinuclear Metal Acetate Complexes: Synthesis, Electronic Structure, and Magnetic Coupling. <i>Inorganic Chemistry</i> , 2016, 55, 1683-1696. | 1.9 | 25 |
| 10308 | Structure, Ionization, and Fragmentation of Neutral and Positively Charged Hydrogenated Carbon Clusters: C_nH_m ($n = 1-5$, $m = 1-10$). <i>Journal of Physical Chemistry A</i> , 2016, 120, 10000-10006. | 0.0 | 0 |
| 10309 | $\text{Pt}^{\text{II}}\text{H}$ Nonclassical Interaction in Water-Dissolved Pt(II) Complexes: Coaction of Electronic Effects with Solvent-Assisted Stabilization. <i>Inorganic Chemistry</i> , 2016, 55, 3252-3264. | 1.9 | 13 |
| 10310 | Roles of Water Molecules in Modulating the Reactivity of Dioxygen-Bound Cu-ZSM-5 toward Methane: A Theoretical Prediction. <i>ACS Catalysis</i> , 2016, 6, 2487-2495. | 5.5 | 54 |
| 10311 | An experimental NEXAFS and computational TDDFT and $\hat{\Gamma}$ -DFT study of the gas-phase core excitation spectra of nitroxide free radical TEMPO and its analogues. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 10207-10217. | 1.3 | 21 |
| 10312 | Synthesis of 1,5-disubstituted tetrazoles containing a fragment of the anticancer drug imatinib via a microwave-assisted Ugi-azide reaction. <i>Monatshefte für Chemie</i> , 2016, 147, 1277-1290. | 0.9 | 21 |
| 10313 | Two-State Reactivity in Low-Valent Iron-Mediated C-H Activation and the Implications for Other First-Row Transition Metals. <i>Journal of the American Chemical Society</i> , 2016, 138, 3715-3730. | 6.6 | 136 |
| 10314 | Theoretical Study of Spin Crossover in 30 Iron Complexes. <i>Inorganic Chemistry</i> , 2016, 55, 2717-2727. | 1.9 | 139 |
| 10315 | Simulation of Two-Dimensional Infrared Spectroscopy of Peptides Using Localized Normal Modes. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1905-1918. | 2.3 | 20 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10316 | Novel and potent Lewis acid catalyst: Br ₂ -catalyzed Friedel-Crafts reactions of naphthols with aldehydes. <i>Synthetic Communications</i> , 2016, 46, 379-385. | 1.1 | 8 |
| 10317 | Reaction dynamics of CO_2 in aqueous amines from ab initio molecular dynamics: 2-amino-2-methyl-1,3-propanediol (AMPD) compared to monoethanolamine (MEA). <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 13 |
| 10318 | Comparison of the Fourier and Discrete-Variable-Representation Methods in the Numerical Solution of Multidimensional Schrödinger Equations. <i>Journal of Applied Spectroscopy</i> , 2016, 82, 893-900. | 0.3 | 17 |
| 10319 | Biomolecule Analogues 2-Hydroxypyridine and 2-Pyridone Base Pairing on Ice Nanoparticles. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4720-4730. | 1.1 | 11 |
| 10320 | Polymer Optical Constants from Long-Range Corrected DFT Calculations. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2507-2516. | 1.2 | 8 |
| 10321 | Experimental and computational approaches of a novel methyl (2E)-2-[N-(2-formylphenyl)(4-methylbenzene)sulfonamido]methyl]-3-(4-chlorophenyl)prop-2-enoate: A potential antimicrobial agent and an inhibition of penicillin-binding protein. <i>Journal of Molecular Structure</i> , 2016, 1115, 33-54. | 1.8 | 18 |
| 10322 | Electronic Structure of a Cu ^{II} Alkoxide Complex Modeling Intermediates in Copper-Catalyzed Alcohol Oxidations. <i>Journal of the American Chemical Society</i> , 2016, 138, 4132-4145. | 6.6 | 12 |
| 10323 | Application of ⁹³ Nb NMR spectroscopy to (silox) ₃ Nb(Xn/Lm) complexes (silox = tBu ₃ SiO): Where does (silox) ₃ Nb(NN)Nb(silox) ₃ appear?. <i>Polyhedron</i> , 2016, 103, 105-114. | 1.0 | 12 |
| 10324 | Crystal solvates of zinc(II) bis(dipyrinates) with triethylamine: composition, stability and spectral-luminescent properties. <i>Journal of Coordination Chemistry</i> , 2016, 69, 901-914. | 0.8 | 9 |
| 10325 | Understanding anionic Chugaev elimination in pericyclic tetracene formation. <i>Tetrahedron</i> , 2016, 72, 1686-1689. | 1.0 | 3 |
| 10326 | Influence of vacancies on GaN/AlN interface characteristics. <i>Proceedings of SPIE</i> , 2016, , . | 0.8 | 0 |
| 10327 | Theoretical investigation of [Ru(tpy) ₂] ²⁺ , [Ru(tpy)(bpy)(H ₂ O)] ²⁺ and [Ru(tpy)(bpy)(Cl)] ⁺ complexes in acetone revisited: Inclusion of strong spin-orbit couplings to quantum chemistry calculations. <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650001. | 1.8 | 1 |
| 10328 | Investigation of Electrolyte Concentration Effects on the Performance of Lithium-Oxygen Batteries. <i>Journal of Physical Chemistry C</i> , 2016, 120, 5949-5957. | 1.5 | 22 |
| 10329 | Insights into the mechanism of silver-catalyzed decarboxylative fluorination. <i>Computational and Theoretical Chemistry</i> , 2016, 1082, 11-20. | 1.1 | 26 |
| 10330 | Unraveling innate substrate control in site-selective palladium-catalyzed C-H heterocycle functionalization. <i>Chemical Science</i> , 2016, 7, 3900-3909. | 3.7 | 58 |
| 10331 | Palladium-atom catalyzed formic acid decomposition and the switch of reaction mechanism with temperature. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 10005-10017. | 1.3 | 26 |
| 10332 | New Insight into the Nature of Bonding in the Dimers of Lappert's Stannylene and Its Ge Analogs: A Quantum Mechanical Study. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1696-1704. | 2.3 | 16 |
| 10333 | The S66x8 benchmark for noncovalent interactions revisited: explicitly correlated ab initio methods and density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20905-20925. | 1.3 | 182 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10334 | Interplay between C-H \cdots O, O-H \cdots X (X=C, F, Cl) and H \cdots O \cdots Y (C, Cl, F) interactions in methane-water and halogen substituted methane-water complexes: Theoretical investigations of structure and energy. Computational and Theoretical Chemistry, 2016, 1083, 19-30. | 1.1 | 13 |
| 10335 | Donor-driven conformational flexibility in a real-life catalytic dicopper(μ -peroxo) complex. Physical Chemistry Chemical Physics, 2016, 18, 6430-6440. | 1.3 | 21 |
| 10336 | Adsorption of complex silver cyanides on Ag(111). Quantum chemical consideration. Russian Journal of Electrochemistry, 2016, 52, 63-70. | 0.3 | 3 |
| 10337 | Theory and Modeling of Asymmetric Catalytic Reactions. Accounts of Chemical Research, 2016, 49, 750-762. | 7.6 | 149 |
| 10338 | Accelerating <i>Ab Initio</i> Path Integral Simulations via Imaginary Multiple-Timestepping. Journal of Chemical Theory and Computation, 2016, 12, 1627-1638. | 2.3 | 12 |
| 10339 | Crystal Structure and Theoretical Analysis of Green Gold Au ₃₀ (S-t-Bu) ₁₈ Nanomolecules and Their Relation to Au ₃₀ S(S-t-Bu) ₁₈ . Journal of Physical Chemistry C, 2016, 120, 6256-6261. | 1.5 | 72 |
| 10340 | Dependence of cobaltocenium diffusion in ionic liquids on the alkyl chain length of 1-alkyl-3-methylimidazolium cations. Physical Chemistry Chemical Physics, 2016, 18, 3558-3566. | 1.3 | 10 |
| 10341 | Identification of Ion-Pair Structures in Solution by Vibrational Stark Effects. Journal of Physical Chemistry B, 2016, 120, 1149-1157. | 1.2 | 22 |
| 10342 | Exploration of some refinements to geometry optimization methods. Theoretical Chemistry Accounts, 2016, 135, 1. | 0.5 | 15 |
| 10343 | Polyhedral dinickelaboranes as analogues of the dicarbaboranes. Polyhedron, 2016, 110, 31-36. | 1.0 | 2 |
| 10344 | Silane-initiated nucleation in chemically active plasmas: validation of density functionals, mechanisms, and pressure-dependent variational transition state calculations. Physical Chemistry Chemical Physics, 2016, 18, 10097-10108. | 1.3 | 28 |
| 10345 | Critical Assessment of TD-DFT for Excited States of Open-Shell Systems: I. Doublet-Doublet Transitions. Journal of Chemical Theory and Computation, 2016, 12, 238-260. | 2.3 | 35 |
| 10346 | Mechanism of Rh ₂ (II)-Catalyzed Indole Formation: The Catalyst Does Not Control Product Selectivity. Journal of the American Chemical Society, 2016, 138, 487-490. | 6.6 | 53 |
| 10347 | Electronic Structure Description of a Doubly Oxidized Bimetallic Cobalt Complex with Proradical Ligands. Inorganic Chemistry, 2016, 55, 762-774. | 1.9 | 30 |
| 10348 | Palladium-Silver Cooperativity in an Aryl Amination Reaction through C-H Functionalization. ACS Catalysis, 2016, 6, 696-708. | 5.5 | 68 |
| 10349 | A comparative study of the xDH-PBE0 and DSD-PBEPBE-D3BJ doubly hybrid density functionals. Molecular Physics, 2016, 114, 1207-1217. | 0.8 | 10 |
| 10350 | Predicting Near Edge X-ray Absorption Spectra with the Spin-Free Exact-Two-Component Hamiltonian and Orthogonality Constrained Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 144-156. | 2.3 | 42 |
| 10351 | Molecular simulation of low temperature argon adsorption in several models of IRMOF-1 with defects and structural disorder. Dalton Transactions, 2016, 45, 4203-4212. | 1.6 | 25 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10352 | Optical Rotation from Coupled Cluster and Density Functional Theory: The Role of Basis Set Convergence. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 535-548. | 2.3 | 21 |
| 10353 | Bifunctional hydrophobic ionic liquids: facile synthesis by thiol-ene click-chemistry. <i>Green Chemistry</i> , 2016, 18, 2443-2452. | 4.6 | 30 |
| 10354 | N-Heterocyclic carbene adducts to [Cp ² Fe] ₂ : synthesis and molecular and electronic structure. <i>Inorganic Chemistry Frontiers</i> , 2016, 3, 250-262. | 3.0 | 20 |
| 10355 | Mechanism, chemoselectivity and enantioselectivity for the rhodium-catalyzed desymmetric synthesis of hydrobenzofurans: a theoretical study. <i>Organic Chemistry Frontiers</i> , 2016, 3, 209-216. | 2.3 | 21 |
| 10356 | Anomalous Size Dependence of Optical Properties in Black Phosphorus Quantum Dots. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 370-375. | 2.1 | 99 |
| 10357 | Oxidation triggers extensive conjugation and unusual stabilization of two di-heme dication diradical intermediates: role of bridging group for electronic communication. <i>Chemical Science</i> , 2016, 7, 1212-1223. | 3.7 | 44 |
| 10358 | Calculation of low bandgap homopolymers: Comparison of TD-DFT methods with experimental oligomer series. <i>Chemical Physics Letters</i> , 2016, 645, 169-173. | 1.2 | 26 |
| 10359 | Butadiene dyes based on 3-(dicyanomethylidene)indan-1-one and 1,3-bis(dicyanomethylidene)indane: synthesis, characterization and solvatochromic behaviour. <i>RSC Advances</i> , 2016, 6, 6858-6867. | 1.7 | 11 |
| 10360 | Synthesis, isomerization and biological activity of novel 2-selenohydantoin derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 802-811. | 1.4 | 25 |
| 10361 | Influence of the supramolecular order on the electrical properties of 1D coordination polymers based materials. <i>Nanoscale</i> , 2016, 8, 2386-2394. | 2.8 | 8 |
| 10362 | Computationally designed zirconium organometallic catalyst for direct epoxidation of alkenes without allylic H atoms: aromatic linkage eliminates formation of inert octahedral complexes. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1. | 0.5 | 3 |
| 10363 | Transition States of Vicinal Diamine-Catalyzed Aldol Reactions. <i>Journal of the American Chemical Society</i> , 2016, 138, 503-506. | 6.6 | 24 |
| 10364 | Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules III: A Benchmark of <i>GW</i> Methods. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 615-626. | 2.3 | 154 |
| 10365 | MN15-L: A New Local Exchange-Correlation Functional for Kohn-Sham Density Functional Theory with Broad Accuracy for Atoms, Molecules, and Solids. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1280-1293. | 2.3 | 364 |
| 10366 | Bicosahedral metallaboranes: aromaticity in metal derivatives of three-dimensional analogues of naphthalene. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11707-11710. | 1.3 | 3 |
| 10367 | Contact Ion Pairs on a Protonated Azamacrocyclic: the Role of the Anion Basicity. <i>Journal of the American Society for Mass Spectrometry</i> , 2016, 27, 615-621. | 1.2 | 3 |
| 10368 | A further look at π -delocalization and hydrogen bonding in 2-arylmalondialdehydes. <i>Tetrahedron</i> , 2016, 72, 95-104. | 1.0 | 10 |
| 10369 | U ^y Stretching Vibrations as a Quantitative Measure of the Equatorial Bond Covalency in Uranyl Complexes: A Quantum-Chemical Investigation. <i>Inorganic Chemistry</i> , 2016, 55, 573-583. | 1.9 | 53 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10370 | Theoretical analysis of NMR shieldings in XSe and XTe (X = Si, Ge, Sn and Pb): the spin-rotation constant saga. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3112-3123. | 1.3 | 5 |
| 10371 | Exploring the role of the 3-center-4-electron bond in hypervalent λ^3 -iodanes using the methodology of domain averaged Fermi holes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 846-856. | 1.3 | 15 |
| 10372 | Elaboration, structural, vibrational and optical investigation of a two-dimensional self-assembled organic-inorganic hybrid compound. <i>Journal of Luminescence</i> , 2016, 173, 213-217. | 1.5 | 25 |
| 10373 | Synthesis, characterization and molecular modelling of a novel dipyridamole supramolecule - X-ray structure, quantum mechanics and molecular dynamics study to comprehend the hydrogen bond structure-activity relationship. <i>Journal of Molecular Structure</i> , 2016, 1105, 194-204. | 1.8 | 13 |
| 10374 | Synthesis and Characterization of Tetramethylethylenediamine-Based Hypergolic Ionic Liquids. <i>Journal of Energetic Materials</i> , 2016, 34, 138-151. | 1.0 | 11 |
| 10375 | Role of Amine Functionality for CO ₂ Chemisorption on Silica. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1988-1995. | 1.2 | 92 |
| 10376 | Tetrahedral tilting and ferroelectricity in Bi ₂ AO ₅ (A=Si, Ge) from first principles calculations. <i>Journal of Solid State Chemistry</i> , 2016, 235, 68-75. | 1.4 | 33 |
| 10377 | Chemical constituents of <i>Ligularia alticola</i> Worosch. leaves and their biological activities. <i>Phytochemistry Letters</i> , 2016, 15, 46-52. | 0.6 | 9 |
| 10378 | Oxidative Dimerization of Triarylaminines Promoted by WCl ₆ , Including the Solid State Isolation and the Crystallographic Characterization of a Triphenylammonium Salt. <i>Inorganic Chemistry</i> , 2016, 55, 887-893. | 1.9 | 15 |
| 10379 | Mitochondria-Targeted Fluorescent Probe for Imaging Hydrogen Peroxide in Living Cells. <i>Analytical Chemistry</i> , 2016, 88, 1455-1461. | 3.2 | 168 |
| 10380 | Cyclopentadienylironphosphacarboranes: fragility of polyhedral edges in the 11-vertex system. <i>RSC Advances</i> , 2016, 6, 1122-1128. | 1.7 | 3 |
| 10381 | Analytic calculations of anharmonic infrared and Raman vibrational spectra. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4201-4215. | 1.3 | 27 |
| 10382 | The infrared spectra of polycyclic aromatic hydrocarbons with C _n H _m side groups. <i>Chemical Physics</i> , 2016, 465-466, 17-27. | 0.9 | 2 |
| 10383 | Linear and Nonlinear Optical Response in Silver Nanoclusters: Insight from a Computational Investigation. <i>Journal of Physical Chemistry A</i> , 2016, 120, 507-518. | 1.1 | 31 |
| 10384 | Orientation of Cyano-Substituted Bipyridine Re(I) λ^3 -Tricarbonyl Electrocatalysts Bound to Conducting Au Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1657-1665. | 1.5 | 46 |
| 10385 | Electron Paramagnetic Resonance Study of the Interaction of Surface Titanium Species with AlR ₃ Cocatalyst in Supported Ziegler-Natta Catalysts with a Low Titanium Content. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1121-1129. | 1.5 | 16 |
| 10386 | Synthesis and physical properties of tolane liquid crystals containing 2,3-difluorophenylene and terminated by a tetrahydropyran moiety. <i>Liquid Crystals</i> , 2016, 43, 564-572. | 0.9 | 18 |
| 10387 | Photoinduced alignment of polymerisable liquid crystals on photoreactive polymers containing 2,6-bis(benzylidene)-1-cyclohexanone units in the main chain. <i>Liquid Crystals</i> , 2016, 43, 587-597. | 0.9 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 10388 | New trans-dichloropalladium(II) complexes of 7-azaindole: Crystal and molecular structures, FT-IR, FT-Raman and DFT studies. <i>Journal of Molecular Structure</i> , 2016, 1103, 202-211. | 1.8 | 14 |
| 10389 | Pyrazole based solid state emissive NLOphores with TICT characteristics: Synthesis, DFT and TDDFT studies. <i>Dyes and Pigments</i> , 2016, 126, 62-75. | 2.0 | 38 |
| 10390 | Tetra-cationic imidazoliumyl-substituted phosphorus-sulfur heterocycles from a cationic organophosphorus sulfide. <i>Chemical Communications</i> , 2016, 52, 2023-2026. | 2.2 | 18 |
| 10391 | Insights into structural and dynamical features of water at halloysite interfaces probed by DFT and classical molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2164-2174. | 1.3 | 37 |
| 10392 | A zinc(II) amidine complex: tandem synthesis, structure, and self assembly. <i>Journal of Coordination Chemistry</i> , 2016, 69, 112-122. | 0.8 | 2 |
| 10393 | Effect of high-voltage electric field on formaldehyde diffusion within building materials. <i>Building and Environment</i> , 2016, 95, 372-380. | 3.0 | 9 |
| 10394 | 5,7-Bis(2-arylethenyl)-6H-1,4-diazepine-2,3-dicarbonitriles: synthesis, and experimental and theoretical evaluation of the effects of substituents at 5,6,7-positions on the molecular configuration and spectral properties. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 1138-1146. | 1.5 | 10 |
| 10395 | A dual-responsive nanocapsule via disulfide-induced self-assembly for therapeutic agent delivery. <i>Chemical Science</i> , 2016, 7, 1846-1852. | 3.7 | 92 |
| 10396 | Aggregation induced emissive carbazole-based push pull NLOphores: Synthesis, photophysical properties and DFT studies. <i>Dyes and Pigments</i> , 2016, 124, 82-92. | 2.0 | 46 |
| 10397 | Can DFT and ab initio methods describe all aspects of the potential energy surface of cycloreversion reactions?. <i>Molecular Physics</i> , 2016, 114, 21-33. | 0.8 | 21 |
| 10398 | Understanding and predicting the orientation of heteroleptic phosphors in organic light-emitting materials. <i>Nature Materials</i> , 2016, 15, 85-91. | 13.3 | 217 |
| 10399 | Terahertz absorption spectra and potential energy distribution of liquid crystals. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 153, 741-745. | 2.0 | 5 |
| 10400 | Synthesis, DFT calculations and characterisation of new mixed Pt(II) complexes with 3-thiolanespiro-5 ² -1-hydantoin and 4-thio-1H-tetrahydropyranspiro-5 ² -hydantoin. <i>Chemical Papers</i> , 2016, 70, . | 1.0 | 5 |
| 10401 | Theoretical insight into the mechanisms of the synthesis of chiral gold(I)-aminocarbene complexes. <i>Journal of Organometallic Chemistry</i> , 2016, 801, 24-29. | 0.8 | 3 |
| 10402 | A novel method for the calculation of bond stretching force constants of diatomic molecules. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 154, 103-107. | 2.0 | 12 |
| 10403 | Infrared, Raman and NMR spectral analysis, vibrational assignments, normal coordinate analysis, and quantum mechanical calculations of 2-Amino-5-ethyl-1,3,4-thiadiazole. <i>Journal of Molecular Structure</i> , 2016, 1103, 70-81. | 1.8 | 11 |
| 10404 | Theoretical and experimental investigations on molecular structure of bis(2-methoxy-4-allylphenyl)oxalate. <i>Journal of Molecular Structure</i> , 2016, 1103, 156-165. | 1.8 | 7 |
| 10405 | Computational and carbon-13 NMR studies of Pt-C bonds in Pt-C-P pincer complexes. <i>Dalton Transactions</i> , 2016, 45, 2095-2101. | 1.6 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10406 | Electronic structure and spectroscopy of homoleptic compounds of dimolybdenum using TDDFT. Canadian Journal of Chemistry, 2016, 94, 20-27. | 0.6 | 0 |
| 10407 | Enhanced brightness of 2,6-diphenylthiazolo[4,5-b]pyrazines by introducing double electron donating groups. Journal of Photochemistry and Photobiology A: Chemistry, 2016, 314, 93-95. | 2.0 | 6 |
| 10408 | Molecular structure and vibrational spectroscopic studies of prothionamide by density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 152, 262-271. | 2.0 | 4 |
| 10409 | Elucidating the mechanism responsible for anomalous thermal expansion in a metal-organic framework. Dalton Transactions, 2016, 45, 4141-4149. | 1.6 | 5 |
| 10410 | Water soluble chromone Schiff base derivatives as fluorescence receptor for aluminium(III). Supramolecular Chemistry, 2017, 29, 1-7. | 1.5 | 27 |
| 10411 | Rotationally averaged linear absorption spectra beyond the electric-dipole approximation. Molecular Physics, 2017, 115, 63-74. | 0.8 | 24 |
| 10412 | A COSMO-based approach to computer-aided mixture design. Chemical Engineering Science, 2017, 159, 93-105. | 1.9 | 51 |
| 10413 | Assessing frequency-dependent site polarisabilities in linear response polarisable embedding. Molecular Physics, 2017, 115, 39-47. | 0.8 | 12 |
| 10414 | The acetaminophen metabolite N-acetyl-p-benzoquinone imine (NAPQI) inhibits glutathione synthetase <i>in vitro</i> ; a clue to the mechanism of 5-oxoprolinuric acidosis?. Xenobiotica, 2017, 47, 164-175. | 0.5 | 16 |
| 10415 | On the performance of DFT/MRCI-R and MR-MP2 in spin-orbit coupling calculations on diatomics and polyatomic organic molecules. Molecular Physics, 2017, 115, 109-137. | 0.8 | 14 |
| 10416 | Polynuclear cage-like Au(μ_3) phosphane complexes based on a S_2 template: observation of multiple luminescence in coordinated polyaromatic systems. Dalton Transactions, 2017, 46, 2516-2523. | 1.6 | 14 |
| 10417 | Structure and stability of clusters of \hat{I}^2 -alanine in the gas phase: importance of the nature of intermolecular interactions. Physical Chemistry Chemical Physics, 2017, 19, 5465-5476. | 1.3 | 6 |
| 10418 | Mechanistic study on silver-catalyzed direct amination of unactivated C-H bond. Journal of Organometallic Chemistry, 2017, 832, 1-8. | 0.8 | 7 |
| 10419 | High-pressure synthesis and crystal structure of $In_3B_5O_{12}$. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2017, 72, 69-76. | 0.3 | 6 |
| 10420 | Reactions of Osmium Carbene Complexes $OsCl_3(\eta^5-CR)(PPh_3)_2$ ($R =$ Tj ETQqO O O rgBT /Overl 36, 657-664. | 1.1 | 7 |
| 10421 | Direct evidence for high Na^{+} mobility and high voltage structural processes in $P2-Na_x[Li_yNi_zMn_{1-\hat{a}}\hat{y}\hat{z}]O_2$ ($x, y, z \hat{\%} 1$) cathodes from solid-state NMR and DFT calculations. Journal of Materials Chemistry A, 2017, 5, 4129-4143. | 5.2 | 105 |
| 10422 | Combined First-Principles Calculations and Experimental Study of the Phonon Modes in the Multiferroic Compound GeV_4S_8 . Journal of Physical Chemistry C, 2017, 121, 3522-3529. | 1.5 | 10 |
| 10423 | Molecular Doping of a High Mobility Diketopyrrolopyrrole "Dithienylthieno[3,2-b]thiophene Donor-Acceptor Copolymer with F6TCNNQ. Macromolecules, 2017, 50, 914-926. | 2.2 | 66 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10424 | Mechanism and Origin of Et ₂ Al(OEt)-Induced Chemoselectivity of Nickel-Catalyzed Three-Component Coupling of One Diketene and Two Alkynes. ACS Catalysis, 2017, 7, 1886-1896. | 5.5 | 38 |
| 10425 | Switching between Inner- and Outer-Sphere PCET Mechanisms of Small-Molecule Activation: Superoxide Dismutation and Oxygen/Superoxide Reduction Reactivity Deriving from the Same Manganese Complex. Journal of the American Chemical Society, 2017, 139, 1472-1484. | 6.6 | 37 |
| 10426 | A promising lead-free fluoride carbonate SHG material designed from a theoretical perspective. Dalton Transactions, 2017, 46, 2635-2642. | 1.6 | 15 |
| 10427 | Theoretical insight into the mechanisms and regioselectivity for the borylation reactions of aryl 2-pyridyl ethers catalyzed by rhodium. Journal of Organometallic Chemistry, 2017, 830, 175-180. | 0.8 | 2 |
| 10428 | An unusual asymmetric pseudomacrocyclic free base ligand and nickel(II) chelate: X-ray crystallographic and DFT studies. Polyhedron, 2017, 124, 22-29. | 1.0 | 4 |
| 10429 | Density functional theory is straying from the path toward the exact functional. Science, 2017, 355, 49-52. | 6.0 | 711 |
| 10430 | Investigation of a new bis(carboxylate)triazole-based anchoring ligand for dye solar cell chromophore complexes. Dalton Transactions, 2017, 46, 1520-1530. | 1.6 | 17 |
| 10431 | DFT study of water adsorption on lignite molecule surface. Journal of Molecular Modeling, 2017, 23, 27. | 0.8 | 30 |
| 10432 | An empirical force field for the simulation of the vibrational spectroscopy of carbon nanomaterials. Carbon, 2017, 113, 299-308. | 5.4 | 12 |
| 10433 | Distributions of therapeutically promising neurosteroids in cellular membranes. Chemistry and Physics of Lipids, 2017, 203, 78-86. | 1.5 | 3 |
| 10434 | Designing Mg ₇ cluster-assembled two dimensional crystal. FlatChem, 2017, 1, 57-59. | 2.8 | 4 |
| 10435 | Quantum control with smoothly varying pulses: general theory and application to charge migration. Journal of Modern Optics, 2017, 64, 1031-1041. | 0.6 | 21 |
| 10436 | TD-DFT Study of Absorption and Emission Spectra of 2-(2-Aminophenyl)benzothiazole Derivatives in Water. Journal of Fluorescence, 2017, 27, 745-754. | 1.3 | 7 |
| 10437 | A Density functional theory study of the sensitivity of two-dimensional BN nanosheet to nerve agents cyclosarin and tabun. Thin Solid Films, 2017, 623, 157-163. | 0.8 | 71 |
| 10438 | Pyrene based D π A architectures: synthesis, density functional theory, photophysics and electron transfer dynamics. Physical Chemistry Chemical Physics, 2017, 19, 3125-3135. | 1.3 | 27 |
| 10439 | Systematic Quantum Mechanical Region Determination in QM/MM Simulation. Journal of Chemical Theory and Computation, 2017, 13, 563-576. | 2.3 | 72 |
| 10440 | Evaluating Electronic Couplings for Excited State Charge Transfer Based on Maximum Occupation Method I ^{SCF} Quasi-Adiabatic States. Journal of Chemical Theory and Computation, 2017, 13, 843-851. | 2.3 | 17 |
| 10441 | Rational Design of a Low-Cost, High-Performance Metal-Organic Framework for Hydrogen Storage and Carbon Capture. Journal of Physical Chemistry C, 2017, 121, 1171-1181. | 1.5 | 84 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10442 | Quantum-chemical insights from deep tensor neural networks. <i>Nature Communications</i> , 2017, 8, 13890. | 5.8 | 884 |
| 10443 | 1,3-Dipolar cycloadditions with meso-tetraarylchlorins " site selectivity and mixed bisadducts. <i>Organic Chemistry Frontiers</i> , 2017, 4, 534-544. | 2.3 | 13 |
| 10444 | Conformation and Dynamics of Human Urotensin II and Urotensin Related Peptide in Aqueous Solution. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 298-310. | 2.5 | 12 |
| 10445 | Chitosan Film Containing an Iron Complex: Synthesis and Prospects for Heterocyclic Aromatic Amines (HAAs) Recognition. <i>Journal of Agricultural and Food Chemistry</i> , 2017, 65, 1387-1394. | 2.4 | 9 |
| 10446 | Potential Functional Embedding Theory at the Correlated Wave Function Level. 2. Error Sources and Performance Tests. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1081-1093. | 2.3 | 16 |
| 10447 | Formation of Dinuclear Iridium Complexes by NHC-Supported C-H Bond Activation. <i>Organometallics</i> , 2017, 36, 699-707. | 1.1 | 15 |
| 10448 | Predicting bond dissociation energy and bond length for bimetallic diatomic molecules: a challenge for electronic structure theory. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5839-5854. | 1.3 | 21 |
| 10449 | Polarizable Force Fields for CO ₂ and CH ₄ Adsorption in M-MOF-74. <i>Journal of Physical Chemistry C</i> , 2017, 121, 4659-4673. | 1.5 | 87 |
| 10450 | Accurate description of the electronic structure of organic semiconductors by GW methods. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 103003. | 0.7 | 26 |
| 10451 | Evaluation of DFT-D3 dispersion corrections for various structural benchmark sets. <i>Journal of Chemical Physics</i> , 2017, 146, 044115. | 1.2 | 23 |
| 10452 | Auxiliary Density Functional Theory: From Molecules to Nanostructures. , 2017, , 795-860. | | 6 |
| 10453 | Photoactive Semiconducting Oxides for Energy and Environment: Experimental and Theoretical Insights. , 2017, , 983-1030. | | 0 |
| 10454 | Tailoring the Schiff base photoswitching " a non-adiabatic molecular dynamics study of substituent effect on excited state proton transfer. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5318-5325. | 1.3 | 30 |
| 10455 | An averaged polarizable potential for multiscale modeling in phospholipid membranes. <i>Journal of Computational Chemistry</i> , 2017, 38, 601-611. | 1.5 | 12 |
| 10456 | Computational Kinetics by Variational Transition-State Theory with Semiclassical Multidimensional Tunneling: Direct Dynamics Rate Constants for the Abstraction of H from CH ₃ OH by Triplet Oxygen Atoms. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1693-1707. | 1.1 | 17 |
| 10457 | Quantum mechanics investigation of initial reaction pathways and early ring-opening reactions in thermal decomposition of liquid-phase RDX. <i>Combustion and Flame</i> , 2017, 178, 7-20. | 2.8 | 40 |
| 10458 | New cyclometalated iridium(III) dye chromophore complexes for p-type dye-sensitised solar cells. <i>Dyes and Pigments</i> , 2017, 140, 269-277. | 2.0 | 30 |
| 10459 | Orientations of nonlocal vibrational modes from combined experimental and theoretical sum frequency spectroscopy. <i>Chemical Physics Letters</i> , 2017, 683, 199-204. | 1.2 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10460 | Theoretical elucidation of the potential possibility of synthesizing arylboronic acids via Rh-catalytic borylations of aryl acetylene and aryl ethylene. <i>Journal of Organometallic Chemistry</i> , 2017, 831, 36-44. | 0.8 | 1 |
| 10461 | Development of Predictive Models of the Kinetics of a Hydrogen Abstraction Reaction Combining Quantum-Mechanical Calculations and Experimental Data. <i>Industrial & Engineering Chemistry Research</i> , 2017, 56, 815-831. | 1.8 | 8 |
| 10462 | Mechanochemical Tuning of Pyrene Absorption Spectrum Using Force Probes. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 727-736. | 2.3 | 8 |
| 10463 | On the multi-reference nature of plutonium oxides: PuO ₂ ²⁺ , PuO ₂ , PuO ₃ and PuO ₂ (OH) ₂ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 4317-4329. | 1.3 | 27 |
| 10464 | DFT and PCM-TD-DFT investigation of the electronic structures and spectra of 5-(3-phenyl-2-propenylidene)-2-thioxo-4-thiazolidinone derivatives. <i>Journal of Molecular Structure</i> , 2017, 1134, 840-850. | 1.8 | 13 |
| 10465 | The Synthesis and Study of Compounds Based on 3,4-Bis(aminofurazano)furoxan. <i>ChemistrySelect</i> , 2017, 2, 688-696. | 0.7 | 11 |
| 10466 | Magnesium-based additives for the cathode slurry to enable high voltage application of lithium-ion batteries. <i>Electrochimica Acta</i> , 2017, 228, 9-17. | 2.6 | 16 |
| 10467 | Phosphorus quantum dots as visible-light photocatalyst for water splitting. <i>Computational Materials Science</i> , 2017, 130, 56-63. | 1.4 | 53 |
| 10468 | Thiolate- π -palladium(σ) or sulfonium- π -palladate(0)? A theoretical study on the mechanism of palladium-catalyzed C-S bond formation reactions. <i>Organic Chemistry Frontiers</i> , 2017, 4, 943-950. | 2.3 | 13 |
| 10469 | Luminescent Pt(σ) complexes featuring imidazolylidene- π -pyridylidene and dianionic bipyrazolate: from fundamentals to OLED fabrications. <i>Journal of Materials Chemistry C</i> , 2017, 5, 1420-1435. | 2.7 | 37 |
| 10470 | Light-Controlled Reversible Modulation of Frontier Molecular Orbital Energy Levels in Trifluoromethylated Diarylethenes. <i>Chemistry - A European Journal</i> , 2017, 23, 3743-3754. | 1.7 | 43 |
| 10471 | Computational study on vapor phase coupling reaction between diiso(thio)cyanates with diamines, diols, and dithiols. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25341. | 1.0 | 2 |
| 10472 | Elucidation of Single Hydrogen Bonds in GTPases via Experimental and Theoretical Infrared Spectroscopy. <i>Biophysical Journal</i> , 2017, 112, 66-77. | 0.2 | 11 |
| 10473 | Theoretical Design of Perylene Diimide Dimers with Different Linkers and Bridged Positions as Promising Non-Fullerene Acceptors for Organic Photovoltaic Cells. <i>Journal of Physical Chemistry C</i> , 2017, 121, 2125-2134. | 1.5 | 50 |
| 10474 | Simulation study on the effects of chemical structure and molecular size on the acceptor strength in poly(3-hexylthiophene)-based copolymer with alternating donor and acceptor for photovoltaic applications. <i>Journal Physics D: Applied Physics</i> , 2017, 50, 065502. | 1.3 | 1 |
| 10475 | Non-Isocyanate Polyurethane Soft Nanoparticles Obtained by Surfactant-Assisted Interfacial Polymerization. <i>Langmuir</i> , 2017, 33, 1959-1968. | 1.6 | 36 |
| 10476 | Chasing the Evasive Fe-O Stretch and the Spin State of the Iron(IV)-Oxo Complexes by Photodissociation Spectroscopy. <i>Journal of the American Chemical Society</i> , 2017, 139, 2757-2765. | 6.6 | 45 |
| 10477 | Density functional theory studies on the conversion of hydroxyheme to iron-verdoheme in the presence of dioxygen. <i>Dalton Transactions</i> , 2017, 46, 2146-2158. | 1.6 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10478 | Stereoisomers of oseltamivir " synthesis, in silico prediction and biological evaluation. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 1828-1841. | 1.5 | 10 |
| 10479 | Absolute Configuration Determination of a Taxol Precursor Based on Raman Optical Activity Spectra. <i>Journal of Physical Chemistry B</i> , 2017, 121, 1544-1551. | 1.2 | 13 |
| 10480 | Insights into selenylation of imidazo[1,2-a]pyridine: synthesis, structural and antimicrobial evaluation. <i>New Journal of Chemistry</i> , 2017, 41, 2919-2926. | 1.4 | 21 |
| 10481 | Structure-activity relationships of fraxamoside as an unusual xanthine oxidase inhibitor. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2017, 32, 345-354. | 2.5 | 21 |
| 10482 | Fallaxosides B 1 and D 3 , triterpene glycosides with novel skeleton types of aglycones from the sea cucumber <i>Cucumaria fallax</i> . <i>Tetrahedron</i> , 2017, 73, 2335-2341. | 1.0 | 10 |
| 10483 | Synthesis and Reactivity of Intramolecularly NHC-Stabilized Germynes and Stannylenes. <i>Organometallics</i> , 2017, 36, 1001-1008. | 1.1 | 15 |
| 10484 | Acid Gas Adsorption on Metal-Organic Framework Nanosheets as a Model of an "All-Surface" Material. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1341-1350. | 2.3 | 23 |
| 10485 | Insights into the enhanced Ce-N triple bond in the HCe-N molecule. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 8216-8222. | 1.3 | 10 |
| 10486 | Development of New Density Functional Approximations. <i>Annual Review of Physical Chemistry</i> , 2017, 68, 155-182. | 4.8 | 51 |
| 10487 | How to computationally calculate thermochemical properties objectively, accurately, and as economically as possible. <i>Pure and Applied Chemistry</i> , 2017, 89, 699-713. | 0.9 | 37 |
| 10488 | A Direct Link from the Gas to the Condensed Phase: A Rotational Spectroscopic Study of 2,2,2-Trifluoroethanol Trimers. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 6289-6293. | 7.2 | 52 |
| 10489 | Computational investigation of fullerene-DNA interactions: Implications of fullerene's size and functionalization on DNA structure and binding energetics. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 74, 177-192. | 1.3 | 6 |
| 10490 | LiTfO: A Highly Efficient Additive for Electrolyte Stabilization in Lithium-Ion Batteries. <i>Chemistry of Materials</i> , 2017, 29, 2254-2263. | 3.2 | 69 |
| 10491 | Electrochemical study of chromium(0) Fischer carbene complexes: Trends in redox potential. <i>Polyhedron</i> , 2017, 127, 323-330. | 1.0 | 5 |
| 10492 | Measuring multi-configurational character by orbital entanglement. <i>Molecular Physics</i> , 2017, 115, 2110-2119. | 0.8 | 49 |
| 10493 | Online Quantification of Criegee Intermediates of α -Pinene Ozonolysis by Stabilization with Spin Traps and Proton-Transfer Reaction Mass Spectrometry Detection. <i>Journal of the American Chemical Society</i> , 2017, 139, 3999-4008. | 6.6 | 29 |
| 10494 | S-Functionalization of 3,5-bis(2-pyridyl)-1,2,4,6-thiatriazine: probing the effect of alkyl chain length in the development of tethered materials. <i>New Journal of Chemistry</i> , 2017, 41, 2268-2276. | 1.4 | 1 |
| 10495 | How computational methods and relativistic effects influence the study of chemical reactions involving Ru-NO complexes?. <i>Journal of Computational Chemistry</i> , 2017, 38, 883-891. | 1.5 | 17 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10496 | Nucleophilic Aromatic Substitution Reactions Described by the Local Electron Attachment Energy. <i>Journal of Organic Chemistry</i> , 2017, 82, 3072-3083. | 1.7 | 38 |
| 10497 | Benchmarking Density Functionals for Chemical Bonds of Gold. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2022-2034. | 1.1 | 23 |
| 10498 | Structure and characterization of physicochemical and magnetic properties of new complex containing monobridged oxygen copper(II) dinuclear cation. <i>Polyhedron</i> , 2017, 127, 144-152. | 1.0 | 5 |
| 10499 | Automatic Reaction Pathway Search via Combined Molecular Dynamics and Coordinate Driving Method. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1351-1361. | 1.1 | 61 |
| 10500 | Mechanistic Insight into the Rh(III)-Catalyzed C-H Activation of 2-Acetyl-1-Arylhydrazines in Water. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1825-1832. | 1.1 | 13 |
| 10501 | Anharmonic, dynamic and functional level effects in far-infrared spectroscopy: Phenol derivatives. <i>Journal of Molecular Spectroscopy</i> , 2017, 342, 4-16. | 0.4 | 10 |
| 10502 | Jahn-Teller and Non-Jahn-Teller Systems Involving CuF_6^{4-} Units: Role of the Internal Electric Field in $\text{Ba}_2\text{ZnF}_6\text{:Cu}^{2+}$ and Other Insulating Systems. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5215-5224. | 1.5 | 17 |
| 10503 | Effect of ortho-substituted aniline on the corrosion protection of aluminum in 2 mol/L H_2SO_4 solution. <i>Canadian Journal of Chemistry</i> , 2017, 95, 612-619. | 0.6 | 10 |
| 10504 | Förster Resonance Energy Transfer between Fluorescent Proteins: Efficient Transition Charge-Based Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 4220-4238. | 1.5 | 11 |
| 10505 | Structural Elucidation of <i>cis</i> / <i>trans</i> Dicafeoylquinic Acid Photoisomerization Using Ion Mobility Spectrometry-Mass Spectrometry. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1381-1388. | 2.1 | 45 |
| 10506 | A Novel n-Type Organosilane-Metal Ion Hybrid of Rhodamine B and Copper Cation for Low-Temperature Thermoelectric Materials. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 10946-10954. | 4.0 | 11 |
| 10507 | Tuning diastereoisomerism in platinum(II) phosphino- and aminothioloato hydrido complexes. <i>New Journal of Chemistry</i> , 2017, 41, 3015-3028. | 1.4 | 1 |
| 10508 | Tightly Bound Double-Caged [60]Fullerene Derivatives with Enhanced Solubility: Structural Features and Application in Solar Cells. <i>Chemistry - an Asian Journal</i> , 2017, 12, 1075-1086. | 1.7 | 7 |
| 10509 | Effects of Multi-Carborane Substitution on the Photophysical and Electron-Accepting Properties of <i>o</i> -Carboranylbenzene Compounds. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 2496-2503. | 1.0 | 15 |
| 10510 | Influence of electron correlation on the electronic and magnetic structures of nitric-oxide-adsorbed manganese phthalocyanine. <i>Chemical Physics Letters</i> , 2017, 675, 15-19. | 1.2 | 3 |
| 10511 | Is a 1,4-Alkyl Shift Involved in the Biosynthesis of Ledol and Viridiflorol?. <i>Journal of Organic Chemistry</i> , 2017, 82, 3957-3959. | 1.7 | 10 |
| 10512 | Lumisterol to Tachysterol Photoisomerization in EPA Glass at 77 K. A Comparative Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2331-2342. | 1.1 | 8 |
| 10513 | Mechanism of Hydrogen-Bonded Complex Formation between Ibuprofen and Nanocrystalline Hydroxyapatite. <i>Langmuir</i> , 2017, 33, 2965-2976. | 1.6 | 31 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10514 | Mechanistic insight into the selective olefin-directed oxidative carbocyclization and borylation by a palladium catalyst: a theoretical study. <i>RSC Advances</i> , 2017, 7, 5013-5018. | 1.7 | 13 |
| 10515 | Energetics of H_2 clusters from density functional and coupled cluster theories. <i>Physical Review B</i> , 2017, 95, . | 1.1 | 2 |
| 10516 | H-bond stabilization of a tautomeric coumarin-pyrazole-pyridine triad generates a PET driven, reversible and reusable fluorescent chemosensor for anion detection. <i>Dyes and Pigments</i> , 2017, 141, 493-500. | 2.0 | 26 |
| 10517 | Improved Accuracy and Efficiency in Quantum Embedding through Absolute Localization. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1503-1508. | 2.3 | 48 |
| 10518 | Assessing Density Functional Theory Approaches for Predicting the Structure and Relative Energy of Salicylideneaniline Molecular Switches in the Solid State. <i>Journal of Physical Chemistry C</i> , 2017, 121, 6898-6908. | 1.5 | 25 |
| 10519 | A new ligand system containing sulfanilamide and quinazolinone fragments: Synthesis, structure, and properties. <i>Russian Journal of General Chemistry</i> , 2017, 87, 66-75. | 0.3 | 0 |
| 10520 | Theoretical approaches for predicting the color of rigid dyes in solution. <i>Journal of Computational Chemistry</i> , 2017, 38, 998-1004. | 1.5 | 17 |
| 10521 | Complexation of Chiral Zinc-Porphyrin Tweezer with Achiral Diamines: Induction and Two-Step Inversion of Interporphyrin Helicity Monitored by ECD. <i>Inorganic Chemistry</i> , 2017, 56, 3849-3860. | 1.9 | 30 |
| 10522 | Computational study on favipiravir adsorption onto undoped- and silicon-decorated C60 fullerenes. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750011. | 1.8 | 25 |
| 10523 | Low-lying Pt _n cluster structures (n = 6–10) from global optimizations based on DFT potential energy surfaces: Sensitivity of the chemical ordering with the functional. <i>Computational and Theoretical Chemistry</i> , 2017, 1107, 136-141. | 1.1 | 15 |
| 10524 | Intermolecular Singlet and Triplet Exciton Transfer Integrals from Many-Body Green's Functions Theory. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1584-1594. | 2.3 | 13 |
| 10525 | Can X-ray constrained Hartree-Fock wavefunctions retrieve electron correlation?. <i>IUCr</i> , 2017, 4, 136-146. | 1.0 | 44 |
| 10526 | Structural and thermochemical studies on CH ₃ SCH ₂ CHO, CH ₃ CH ₂ SCHO, CH ₃ SC(O)CH ₃ and radicals corresponding to loss of H atom. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3688. | 0.9 | 5 |
| 10527 | Combined powder X-ray diffraction data and quantum-chemical calculations in EXPO2014. <i>Powder Diffraction</i> , 2017, 32, S123-S128. | 0.4 | 7 |
| 10528 | Synthesis and Structure of 2,5-Bis[N-(2,6-mesityl)iminomethyl]pyrrolylcobalt(II): Evidence for One-Electron-Oxidized, Redox Noninnocent Ligand Behavior. <i>Inorganic Chemistry</i> , 2017, 56, 3377-3385. | 1.9 | 12 |
| 10529 | Comparison of Implicit and Explicit Solvent Models for the Calculation of Solvation Free Energy in Organic Solvents. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1034-1043. | 2.3 | 180 |
| 10530 | Switching of Förster to Dexter Mechanism of Short-Range Energy Transfer in meso-Anthrylporphyrin. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5941-5948. | 1.5 | 22 |
| 10531 | Barrier heights of hydrogen-transfer reactions with diffusion quantum monte carlo method. <i>Journal of Computational Chemistry</i> , 2017, 38, 798-806. | 1.5 | 16 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10532 | Ligand size dependence of U–N and U–O bond character in a series of uranyl hexaphyrin complexes: quantum chemical simulation and density based analysis. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 7546-7559. | 1.3 | 10 |
| 10533 | Structural and electronic properties of bulk and low-index surfaces of zincblende PtC. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 125002. | 0.7 | 2 |
| 10534 | The PAH Emission Characteristics of the Reflection Nebula NGC 2023. <i>Astrophysical Journal</i> , 2017, 836, 198. | 1.6 | 76 |
| 10535 | Probing Chemical Bonding and Electronic Structures in ThO ⁺ by Anion Photoelectron Imaging and Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2108-2113. | 1.1 | 8 |
| 10536 | Hexacarbalene Structures with 2 <i>n</i> + 8 Skeletal Electrons: Decorating an Aluminum Cube with Carbon Atoms. <i>Organometallics</i> , 2017, 36, 1019-1026. | 1.1 | 2 |
| 10537 | Probing Transient Valence Orbital Changes with Picosecond Valence-to-Core X-ray Emission Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2017, 121, 2620-2626. | 1.5 | 27 |
| 10538 | Comparison of the Optical and Electrochemical Properties of Bi(perylene diimide)s Linked through Ortho and Bay Positions. <i>ACS Omega</i> , 2017, 2, 377-385. | 1.6 | 41 |
| 10539 | Ammonia Oxidation by Abstraction of Three Hydrogen Atoms from a Mo–NH ₃ Complex. <i>Journal of the American Chemical Society</i> , 2017, 139, 2916-2919. | 6.6 | 54 |
| 10540 | Thioether-functionalized picolinium ionic liquids: synthesis, physical properties and computational studies. <i>New Journal of Chemistry</i> , 2017, 41, 1625-1630. | 1.4 | 11 |
| 10541 | Synthesis, theoretical calculation, electrochemistry and total antioxidant capacity of 5-benzoyl-6-phenyl-4-(4-methoxyphenyl)-1,2,3,4-tetrahydro-2-thioxopyrimidine and derivatives. <i>Journal of Molecular Structure</i> , 2017, 1136, 231-243. | 1.8 | 10 |
| 10542 | Fingerprints of Through-Bond and Through-Space Exciton and Charge Ė-Electron Delocalization in Linearly Extended [2.2]Paracyclophanes. <i>Journal of the American Chemical Society</i> , 2017, 139, 3095-3105. | 6.6 | 34 |
| 10543 | Theoretical and antimicrobial activity study for ethyl{4-[3-(1 <i>H</i> -imidazole-1-yl)propyl]-3-methyl-5-oxo-4,5-dihydro-1 <i>H</i> -1,2,4-triazol-1-yl}acetate. <i>Spectroscopy Letters</i> , 2017, 50, 96-101. | 0.5 | 8 |
| 10544 | Quantitative Structure–Activity Relationships for the Nucleophilicity of Trivalent Boron Compounds. <i>Chemistry - A European Journal</i> , 2017, 23, 5066-5075. | 1.7 | 15 |
| 10545 | Sensing properties of monolayer borophane nanosheet towards alcohol vapors: A first-principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 73, 208-216. | 1.3 | 37 |
| 10546 | The Blue-Violet Color of Pentamethylbismuth: A Visible Spin-Orbit Effect. <i>ChemistryOpen</i> , 2017, 6, 15-17. | 0.9 | 4 |
| 10547 | Structural analyses of two new highly distorted octahedral copper(II) complexes with quinoline-type ligands; Hirshfeld, AIM and NBO studies. <i>Polyhedron</i> , 2017, 127, 36-50. | 1.0 | 23 |
| 10548 | Translation of Ligand-Centered Hydrogen Evolution Reaction Activity and Mechanism of a Rhenium-Thiolate from Solution to Modified Electrodes: A Combined Experimental and Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2017, 56, 2177-2187. | 1.9 | 16 |
| 10549 | Synthesis and photophysical properties of phenanthroimidazole–triarylborane dyads: intriguing Ė-turn-on™ sensing mediated by fluoride anions. <i>RSC Advances</i> , 2017, 7, 10345-10352. | 1.7 | 16 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10550 | MP4 Study of the Anharmonic Coupling of the Shared Proton Stretching Vibration of the Protonated Water Dimer in Equilibrium and Transition States. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2151-2165. | 1.1 | 8 |
| 10551 | Testing the CP-correction procedure with different DFT methods on H-bonding complexes of β -carrabiose with water molecules. <i>Journal of Molecular Modeling</i> , 2017, 23, 31. | 0.8 | 8 |
| 10552 | Synthesis of Novel Thiazole Based Carbaldehyde as Potential Sensor for Fluoride Anion and their Spectroscopic Properties. <i>Journal of Fluorescence</i> , 2017, 27, 1117-1128. | 1.3 | 10 |
| 10553 | Luminescent water-soluble cycloplatinated complexes: Structural, photophysical, electrochemical and chiroptical properties. <i>Inorganica Chimica Acta</i> , 2017, 461, 267-274. | 1.2 | 17 |
| 10554 | Theoretical Study on Ruthenium-Catalyzed Hydrocarbamoylative Cyclization of 1,6-Diyne with Dimethylformamide. <i>Organometallics</i> , 2017, 36, 1154-1163. | 1.1 | 6 |
| 10555 | Synthesis of stable cationic waterborne polyurethane with a high solid content: insight from simulation to experiment. <i>RSC Advances</i> , 2017, 7, 13312-13324. | 1.7 | 30 |
| 10556 | HSO_2^+ Formation from Ion-Molecule Reactions of SO_2^+ with Water and Methane: Two Fast Reactions with Reverse Temperature-Dependent Kinetic Trend. <i>Chemistry - A European Journal</i> , 2017, 23, 6772-6780. | 1.7 | 18 |
| 10557 | Itinerant Antiferromagnetism in RuO_2 . <i>Physical Review Letters</i> , 2017, 118, 077201. | 2.9 | 10 |
| 10558 | Molecular dynamics simulations on networks of heparin and collagen. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1119-1130. | 1.5 | 17 |
| 10559 | $[\text{Cu}(\text{H}_2\text{O})_n]^{2+}$ ($n=6$) complexes in solution phase: a DFT hierarchical study. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1. | 0.5 | 18 |
| 10560 | A Benchmark Study of Kinetic Isotope Effects and Barrier Heights for the Finkelstein Reaction. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2311-2321. | 1.1 | 12 |
| 10561 | Multielectron Transfer at Cobalt: Influence of the Phenylazopyridine Ligand. <i>Journal of the American Chemical Society</i> , 2017, 139, 4540-4550. | 6.6 | 34 |
| 10562 | Rapidly accessible rotaxanes utilizing a single amide hydrogen bond templating motif. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 2797-2803. | 1.5 | 15 |
| 10563 | Accurate alkynyl radical structures from density functional calculations without Hartree-Fock exchange. <i>Journal of Chemical Physics</i> , 2017, 146, 054109. | 1.2 | 5 |
| 10564 | Phenanthridine-Containing Pincer-like Amido Complexes of Nickel, Palladium, and Platinum. <i>Inorganic Chemistry</i> , 2017, 56, 3674-3685. | 1.9 | 31 |
| 10565 | Fluorescence intermittency originates from reclustered in two-dimensional organic semiconductors. <i>Nature Communications</i> , 2017, 8, 14521. | 5.8 | 5 |
| 10566 | Detection and identification of Criegee intermediates from the ozonolysis of biogenic and anthropogenic VOCs: comparison between experimental measurements and theoretical calculations. <i>Faraday Discussions</i> , 2017, 200, 559-578. | 1.6 | 12 |
| 10567 | The effect of ring size on the selective carboxylation of cycloalkene oxides. <i>Catalysis Science and Technology</i> , 2017, 7, 1433-1439. | 2.1 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10568 | Engineering of Ruthenium(II) Photosensitizers with Non-Innocent Oxyquinolate and Carboxyamidoquinolate Ligands for Dye-Sensitized Solar Cells. <i>Chemistry - A European Journal</i> , 2017, 23, 7497-7507. | 1.7 | 15 |
| 10569 | When does a functional correctly describe both the structure and the energy of the transition state?. <i>Journal of Molecular Modeling</i> , 2017, 23, 65. | 0.8 | 5 |
| 10570 | Counterion effect on the spin-transition properties of the second generation iron(III) dendrimeric complexes. <i>Inorganica Chimica Acta</i> , 2017, 459, 131-142. | 1.2 | 11 |
| 10571 | X-ray crystallographic analysis and DFT calculations of three π -propylene linker™ dimers linked by one polystep reaction. <i>Journal of Molecular Structure</i> , 2017, 1137, 126-135. | 1.8 | 2 |
| 10572 | Intriguing Indium-salen Complexes as Multicolor Luminophores. <i>Inorganic Chemistry</i> , 2017, 56, 2621-2626. | 1.9 | 28 |
| 10573 | The GlcN6P cofactor plays multiple catalytic roles in the glmS ribozyme. <i>Nature Chemical Biology</i> , 2017, 13, 439-445. | 3.9 | 44 |
| 10574 | Triethylsulfonium and triethylphosphonium cations as novel catalysts for the decomposition process of nitroethyl benzoates. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2017, 192, 1252-1258. | 0.8 | 3 |
| 10575 | Correlation effects on the interelectronic distributions of localized electron pairs. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1. | 0.5 | 1 |
| 10576 | Oxo- and hydroxo-bridged diiron(III) porphyrin dimers: Inorganic and bio-inorganic perspectives and effects of intermacrocylic interactions. <i>Coordination Chemistry Reviews</i> , 2017, 337, 112-144. | 9.5 | 52 |
| 10577 | Influence of Coupling and Embedding Schemes on QM Size Convergence in QM/MM Approaches for the Example of a Proton Transfer in DNA. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1102-1107. | 2.3 | 71 |
| 10578 | Paramagnetic Enhancement of Nuclear Spin-Spin Coupling. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1275-1283. | 2.3 | 8 |
| 10579 | Ultrafast Excited-State Decays in $[\text{Re}(\text{CO})_3(\text{N},\text{N})(\text{L})]^{n+}$: Nonadiabatic Quantum Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1293-1306. | 2.3 | 45 |
| 10580 | Substrate and Lewis Acid Coordination Promote O-O Bond Cleavage of an Unreactive $\text{L}_2\text{Cu}^{\text{II}}(\text{O})_2$ Species to Form $\text{L}_2\text{Cu}^{\text{III}}(\text{O})_2$ Cores with Enhanced Oxidative Reactivity. <i>Journal of the American Chemical Society</i> , 2017, 139, 3186-3195. | 6.6 | 50 |
| 10581 | Unusual (+/-) electro-spray ionization induced fragmentation: Structural elucidation of an in-process synthetic intermediate of doravirine (MK-1439) using liquid chromatography/high-resolution tandem mass spectrometry and two-dimensional nuclear magnetic resonance. <i>Rapid Communications in Mass Spectrometry</i> , 2017, 31, 719-727. | 0.7 | 1 |
| 10582 | Bis-cyclometalated rhodium- and iridium-complexes with the 4,4'-dichloro-2,2'-bipyridine ligand. Evaluation of their photophysical properties and biological activity. <i>Inorganica Chimica Acta</i> , 2017, 463, 36-43. | 1.2 | 15 |
| 10583 | Development and applications of two colorimetric and fluorescent indicators for Hg ²⁺ detection. <i>Journal of Inorganic Biochemistry</i> , 2017, 172, 23-33. | 1.5 | 11 |
| 10584 | Assessing DFT-D3 Damping Functions Across Widely Used Density Functionals: Can We Do Better?. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2043-2052. | 2.3 | 71 |
| 10585 | Salicylaldehyde Hydrazones: Buttressing of Outer-Sphere Hydrogen-Bonding and Copper Extraction Properties. <i>Australian Journal of Chemistry</i> , 2017, 70, 556. | 0.5 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10586 | Is coronene better described by $\langle \text{sc} \rangle \text{C} \langle / \text{sc} \rangle$ lar's aromatic C_6h_6 sextet model or by the AdNDP representation?. Journal of Computational Chemistry, 2017, 38, 1606-1611. | 1.5 | 30 |
| 10587 | Structure-property relationships for covalent triazine-based frameworks: The effect of spacer length on photocatalytic hydrogen evolution from water. Polymer, 2017, 126, 283-290. | 1.8 | 135 |
| 10588 | Tuning the Fe(II/III) Redox Potential in Nonheme Fe(II)-Hydroxo Complexes through Primary and Secondary Coordination Sphere Modifications. Inorganic Chemistry, 2017, 56, 4852-4863. | 1.9 | 35 |
| 10589 | Mechanistic Analysis of Fluorescence Quenching of Reduced Nicotinamide Adenine Dinucleotide by Oxamate in Lactate Dehydrogenase Ternary Complexes. Photochemistry and Photobiology, 2017, 93, 1193-1203. | 1.3 | 14 |
| 10591 | DFT and TD-DFT investigations of organic dye with different C_6H_4 -spacer used for solar cell. Journal of Materials Science: Materials in Electronics, 2017, 28, 9642-9652. | 1.1 | 7 |
| 10592 | Biphenyl- and Fluorene-Based $\langle i \rangle \text{o} \langle /i \rangle$ -Carboranyl Compounds: Alteration of Photophysical Properties by Distortion of Biphenyl Rings. Organometallics, 2017, 36, 1522-1529. | 1.1 | 53 |
| 10593 | Potassium $\langle i \rangle \text{tert} \langle /i \rangle$ -Butoxide-Catalyzed Dehydrogenative $\text{C}-\text{H}$ Silylation of Heteroaromatics: A Combined Experimental and Computational Mechanistic Study. Journal of the American Chemical Society, 2017, 139, 6867-6879. | 6.6 | 160 |
| 10594 | Effect of donor atom identity on metal-binding pharmacophore coordination. Journal of Biological Inorganic Chemistry, 2017, 22, 605-613. | 1.1 | 8 |
| 10595 | Impact of Halogenido Coligands on Magnetic Anisotropy in Seven-Coordinate Co(II) Complexes. Inorganic Chemistry, 2017, 56, 5076-5088. | 1.9 | 57 |
| 10596 | Mechanistic insights into the selective cyclization of indolines with alkynes and alkenes to produce six- and seven-membered 1,7-fused indolines via Rh($\langle \text{sc} \rangle \text{iii} \langle / \text{sc} \rangle$) catalysis: a theoretical study. Organic and Biomolecular Chemistry, 2017, 15, 3938-3946. | 1.5 | 16 |
| 10598 | A Combined Density Functional Theory and Spectrophotometry Study of the Bonding Interactions of $[\text{NpO}(\text{M})_2]^{4+}$ Cation-Cation Complexes. Inorganic Chemistry, 2017, 56, 4788-4795. | 1.9 | 9 |
| 10599 | Electron Paramagnetic Resonance and DFT Analysis of the Effects of Bulky Perfluoroalkyl Substituents on a Vanadyl Perfluoro Phthalocyanine. Zeitschrift Fur Physikalische Chemie, 2017, 231, 887-903. | 1.4 | 8 |
| 10600 | The Dynamics of the Reaction of FeO^+ and H_2 : A Model for Inorganic Oxidation. Angewandte Chemie - International Edition, 2017, 56, 5790-5794. | 7.2 | 18 |
| 10601 | Role of Mediator and Effects of Temperature on $\langle i \rangle \text{ortho} \langle /i \rangle$ - $\text{C}-\text{N}$ Bond Fusion Reactions of Aniline Using Ruthenium Templates: Isolation and Characterization of New Ruthenium Complexes of the in-Situ-Generated Ligands. Inorganic Chemistry, 2017, 56, 4966-4977. | 1.9 | 5 |
| 10602 | Preparation of Phosphorescent Osmium(IV) Complexes with N,N -C_2 - and C,N -C_2 -Pincer Ligands. Organometallics, 2017, 36, 1848-1859. | 1.1 | 34 |
| 10603 | Verification of oligomycin A structure: synthesis and biological evaluation of 33-dehydrooligomycin A. Journal of Antibiotics, 2017, 70, 871-877. | 1.0 | 10 |
| 10604 | On the decay of the triplet state of thionucleobases. Physical Chemistry Chemical Physics, 2017, 19, 12674-12682. | 1.3 | 38 |
| 10605 | Does the ionization potential condition employed in QTP functionals mitigate the self-interaction error?. Journal of Chemical Physics, 2017, 146, 034102. | 1.2 | 22 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10606 | Raman and DRIFT spectra, vibrational assignments and quantum mechanical calculations of centrosymmetric meso -2,3-Dimercaptosuccinic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 183, 275-283. | 2.0 | 7 |
| 10607 | About the nature of halogen bond interaction under the spatial confinement. <i>Journal of Chemical Physics</i> , 2017, 146, 154304. | 1.2 | 2 |
| 10608 | The role of Li ⁺ ions in the gas phase dehydrohalogenation and dehydration reactions of i-C ₃ H ₇ Br and i-C ₃ H ₇ OH molecules studied by radiofrequency-guided ion beam techniques and ab initio methods. <i>Journal of Chemical Physics</i> , 2017, 146, 134301. | 1.2 | 0 |
| 10609 | New Thomimarine E from Marine Isolate of the Fungus <i>Penicillium thomii</i> . <i>Chemistry of Natural Compounds</i> , 2017, 53, 290-294. | 0.2 | 12 |
| 10610 | Can Kohn-Sham density functional theory predict accurate charge distributions for both single-reference and multi-reference molecules?. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12898-12912. | 1.3 | 45 |
| 10611 | Supramolecular nanoparticles of calcitonin and dipeptide for long-term controlled release. <i>Journal of Controlled Release</i> , 2017, 256, 182-192. | 4.8 | 27 |
| 10612 | A Modular Implementation for the Simulation of 1D and 2D Solid-State NMR Spectra of Quadrupolar Nuclei in the Virtual Multifrequency Spectrometer's Draw Graphical Interface. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2215-2229. | 2.3 | 18 |
| 10613 | Solvation Enhances the Distinction between Carboxylated Armchair and Zigzag Single-Wall Carbon Nanotubes (SWNT-COOH). <i>Journal of Physical Chemistry C</i> , 2017, 121, 9516-9527. | 1.5 | 2 |
| 10614 | A new approach to molecular dynamics with non-adiabatic and spin-orbit effects with applications to QM/MM simulations of thiophene and selenophene. <i>Journal of Chemical Physics</i> , 2017, 146, 114101. | 1.2 | 22 |
| 10615 | Lithium and Potassium Complexes with dbn- and dbu-Based Enamido Phosphine Ligands: Syntheses and Applications. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 2671-2681. | 1.0 | 4 |
| 10616 | Mediating gold nanoparticle growth in nanoreactors: Role of template-metal interactions and external energy. <i>Materials Chemistry and Physics</i> , 2017, 196, 92-102. | 2.0 | 1 |
| 10617 | Mechanisms of Carbonyl Activation by BINOL- <i>N</i> -Triflylphosphoramides: Enantioselective Nazarov Cyclizations. <i>ACS Catalysis</i> , 2017, 7, 3466-3476. | 5.5 | 25 |
| 10618 | Effect of Lewis acid bulkiness on the stereoselectivity of Diels-Alder reactions between acyclic dienes and β -enals. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1390-1399. | 2.3 | 29 |
| 10619 | Comparing the performance of TD-DFT and SAC-Cl methods in the description of excited states potential energy surfaces: An excited state proton transfer reaction as case study. <i>Journal of Computational Chemistry</i> , 2017, 38, 1084-1092. | 1.5 | 15 |
| 10620 | Quantitative contribution of molecular orbitals to hydrogen bonding in a water dimer: Electron density projected integral (EDPI) analysis. <i>Chemical Physics Letters</i> , 2017, 678, 98-101. | 1.2 | 5 |
| 10621 | Selective Synthesis and Photophysical Properties of Phosphorescent Heteroleptic Iridium(III) Complexes with Two Different Bidentate Groups and Two Different Monodentate Ligands. <i>Organometallics</i> , 2017, 36, 1743-1755. | 1.1 | 21 |
| 10622 | Electronic σ Tensors in U ^V Complexes: A Computational Study. <i>Chemistry - A European Journal</i> , 2017, 23, 7798-7808. | 1.7 | 4 |
| 10623 | Combined experimental and DFT-TDDFT investigation on anthocyanidins for application in dye-sensitised solar cells. <i>Dyes and Pigments</i> , 2017, 143, 291-300. | 2.0 | 18 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10624 | Tetracobalt-polyoxometalate catalysts for water oxidation: Key mechanistic details. <i>Journal of Catalysis</i> , 2017, 350, 56-63. | 3.1 | 59 |
| 10625 | Infrared spectroscopy of matrix-isolated neutral polycyclic aromatic nitrogen heterocycles: The acridine series. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 181, 286-308. | 2.0 | 22 |
| 10626 | Impact of Conjugation and Hyperconjugation on the Radical Stability of Allylic and Benzylic Systems: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2017, 82, 5731-5742. | 1.7 | 9 |
| 10627 | Sensitivity of Photoelectron Angular Distributions to Molecular Conformations of Anions. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2268-2273. | 2.1 | 18 |
| 10628 | DFT study of CO ₂ and H ₂ O co-adsorption on carbon models of coal surface. <i>Journal of Molecular Modeling</i> , 2017, 23, 187. | 0.8 | 22 |
| 10629 | Coumarin-Pyrazole Hybrid with Red Shifted ESIPT Emission and AIE Characteristics - a Comprehensive Study. <i>Journal of Fluorescence</i> , 2017, 27, 1687-1707. | 1.3 | 15 |
| 10630 | B-DNA model systems in non-terran bio-solvents: implications for structure, stability and replication. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 16969-16978. | 1.3 | 25 |
| 10631 | Atropisomerism and Conformational Equilibria: Impact on PI3K α Inhibition of 2-((6-Amino-9H-purin-9-yl)methyl)-5-methyl-3-(<i>o</i> -tolyl)quinazolin-4(3 <i>H</i>)-one (IC87114) and Its Conformationally Restricted Analogs. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 4304-4315. | 2.9 | 15 |
| 10632 | An octanuclear Schiff-base complex with a Na ₂ Ni ₆ core: structure, magnetism and DFT calculations. <i>RSC Advances</i> , 2017, 7, 25821-25827. | 1.7 | 9 |
| 10633 | Antileishmanial activity study and theoretical calculations for 4-amino-1,2,4-triazole derivatives. <i>Journal of Molecular Structure</i> , 2017, 1144, 80-86. | 1.8 | 34 |
| 10634 | A novel coordination polymer of 7-azaindole-3-carboxylic acid with sodium ions: crystal and molecular structures, vibrational spectra and DFT calculations. <i>Journal of Molecular Structure</i> , 2017, 1144, 338-346. | 1.8 | 11 |
| 10635 | Long-Lived Polypyridyl Based Mononuclear Ruthenium Complexes: Synthesis, Structure, and Azo Dye Decomposition. <i>Inorganic Chemistry</i> , 2017, 56, 6489-6498. | 1.9 | 17 |
| 10636 | Gas-phase reactivity of Cp* group IX metal complexes bearing aromatic N,N ϵ^2 -chelating ligands. <i>New Journal of Chemistry</i> , 2017, 41, 6995-7006. | 1.4 | 12 |
| 10637 | Synergetic effect between spin crossover and luminescence in the [Fe(bpp) ₂][BF ₄] ₂ (bpp =) Tj ETQq1 1 0.784314,rgBT /Overlock 10 FF 2.7 41 | 2.7 | 41 |
| 10638 | Effect of n-propyl substituents on the emission properties of blue phosphorescent iridium(III) complexes. <i>Journal of Chemical Physics</i> , 2017, 146, 174305. | 1.2 | 5 |
| 10639 | Modeling of Bulk Kerogen Porosity: Methods for Control and Characterization. <i>Energy & Fuels</i> , 2017, 31, 6004-6018. | 2.5 | 49 |
| 10640 | Copper-Catalyzed Hydroamination of Allenes: from Mechanistic Understanding to Methodology Development. <i>ACS Catalysis</i> , 2017, 7, 4253-4264. | 5.5 | 50 |
| 10641 | Dissecting the role of dispersion on the quantum topology phase diagram of monosaccharide isomers. <i>Monatshefte für Chemie</i> , 2017, 148, 1269-1276. | 0.9 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 10642 | Diaryl-amino- and Diaryl-boryl-Substituted Donor–Acceptor Pyrene Derivatives: Influence of Substitution Pattern on Their Photophysical Properties. <i>Journal of Organic Chemistry</i> , 2017, 82, 5111-5121. | 1.7 | 47 |
| 10643 | Azaborininones: Synthesis and Structural Analysis of a Carbonyl-Containing Class of Azaborines. <i>Journal of Organic Chemistry</i> , 2017, 82, 5380-5390. | 1.7 | 18 |
| 10644 | Reversible multi-electron redox chemistry of π -conjugated N-containing heteroaromatic molecule-based organic cathodes. <i>Nature Energy</i> , 2017, 2, . | 19.8 | 486 |
| 10645 | Accurate calculations of the noncovalent systems with flat potential energy surfaces: Naphthalene dimer and azulene dimer. <i>Computational and Theoretical Chemistry</i> , 2017, 1112, 52-60. | 1.1 | 4 |
| 10646 | Four faces of the interaction between ions and aromatic rings. <i>Journal of Computational Chemistry</i> , 2017, 38, 1762-1773. | 1.5 | 9 |
| 10647 | Backing of 2-(diethylamino)-N-(2, 6-dimethylphenyl)-acetamide with molecular, electronic and docking studies. <i>Beni-Suef University Journal of Basic and Applied Sciences</i> , 2017, 6, 293-300. | 0.8 | 1 |
| 10648 | Temperature and Pressure Dependences of the Reactions of Fe^{3+} with Methyl Halides CH_3X (X = Cl, Br, I): Experiments and Kinetic Modeling Results. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4058-4068. | 1.1 | 7 |
| 10649 | SAM of Gliotoxin on Gold: A Natural Product Platform for Sugar Recognition based on the Immobilization of <i>Canavalia brasiliensis</i> lectin (ConBr). <i>Electrochimica Acta</i> , 2017, 241, 116-123. | 2.6 | 8 |
| 10650 | Isosorbide telechelic bio-based oligomers. <i>Journal of Polymer Science Part A</i> , 2017, 55, 2178-2189. | 2.5 | 4 |
| 10651 | Antiplasmodial Sesquiterpenoid Lactones from <i>Trichospira verticillata</i> : Structure Elucidation by Spectroscopic Methods and Comparison of Experimental and Calculated ECD Data. <i>Journal of Natural Products</i> , 2017, 80, 1639-1647. | 1.5 | 23 |
| 10652 | An Iodabenzene Story. <i>Journal of the American Chemical Society</i> , 2017, 139, 7124-7129. | 6.6 | 10 |
| 10653 | Assessment of electronic structure methods for the determination of the ground spin states of Fe^{II} , Fe^{III} and Fe^{IV} complexes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13049-13069. | 1.3 | 100 |
| 10654 | The Effect of <i>trans</i> Ligands in the NO–Linkage Reverse Isomerization for Ruthenium–Nitrosyl–Tetraammine Complexes: A DFT Study. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 2951-2954. | 1.0 | 19 |
| 10655 | Clathrate Structure Determination by Combining Crystal Structure Prediction with Computational and Experimental ^{129}Xe NMR Spectroscopy. <i>Chemistry - A European Journal</i> , 2017, 23, 5258-5269. | 1.7 | 18 |
| 10656 | π -(Hetero)aryl–Substituted β -Hydroxyphenalenones: Synthesis and Electronic Properties of Multifunctional Donor–Acceptor Conjugates. <i>Chemistry - A European Journal</i> , 2017, 23, 10551-10558. | 1.7 | 4 |
| 10657 | Combined quantum–mechanical molecular mechanics calculations with NWChem and AMBER: Excited state properties of green fluorescent protein chromophore analogue in aqueous solution. <i>Journal of Computational Chemistry</i> , 2017, 38, 1631-1639. | 1.5 | 3 |
| 10658 | Static (hyper)polarizabilities and absorption spectra of single [2.2]p-cyclophane NO_2/NH_2 substituted from DFT methods. <i>Optical and Quantum Electronics</i> , 2017, 49, 1. | 1.5 | 2 |
| 10659 | HIV-1 Frameshift RNA-Targeted Triazoles Inhibit Propagation of Replication-Competent and Multi-Drug-Resistant HIV in Human Cells. <i>ACS Chemical Biology</i> , 2017, 12, 1674-1682. | 1.6 | 43 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10660 | Anomalous effect of non-alternant hydrocarbons on carbocation and carbanion electronic configurations. <i>Chemical Science</i> , 2017, 8, 4231-4241. | 3.7 | 10 |
| 10661 | Understanding the Difference in Photophysical Properties of Cyclometalated Iridium(III) and Rhodium(III) Complexes by Detailed Time-Dependent Density Functional Theory and Frontier Molecular Orbital Supports. <i>Journal of Physical Chemistry C</i> , 2017, 121, 11632-11642. | 1.5 | 15 |
| 10662 | Developing Comprehensive Computational Parameter Sets To Describe the Performance of Pyridine-Oxazoline and Related Ligands. <i>ACS Catalysis</i> , 2017, 7, 4144-4151. | 5.5 | 76 |
| 10663 | Radical Arylation of Anilines and Pyrroles via Aryldiazotates. <i>Chemistry - A European Journal</i> , 2017, 23, 9647-9656. | 1.7 | 21 |
| 10664 | Ligand exchange adsorption and coordination structure of Pd on γ -MnO ₂ in NaCl solution. <i>Chemical Geology</i> , 2017, 460, 130-137. | 1.4 | 9 |
| 10665 | Magnetic field-induced effects on NMR properties. <i>Journal of Magnetic Resonance</i> , 2017, 281, 1-6. | 1.2 | 5 |
| 10666 | Blue-light induced CO releasing properties of thiourea based manganese(I) carbonyl complexes. <i>Polyhedron</i> , 2017, 131, 13-21. | 1.0 | 11 |
| 10667 | Theoretical simulations for vibrationally-resolved absorption spectra of naphthalenediimide cyclophane derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 183, 339-347. | 2.0 | 7 |
| 10668 | Planar-chiral ferrocenylphosphine-borane complexes featuring agostic-type B σ -H σ E (E = Hg, Sn) interactions. <i>Dalton Transactions</i> , 2017, 46, 6253-6264. | 1.6 | 8 |
| 10669 | The influence of substituents and the environment on the NMR shielding constants of supramolecular complexes based on A σ T and A σ U base pairs. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13496-13502. | 1.3 | 11 |
| 10670 | A theoretical study of ascorbic acid oxidation and HOO^{\bullet} radical scavenging. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 4417-4431. | 1.5 | 108 |
| 10671 | The Dynamics of the Reaction of FeO ⁺ and H ₂ : A Model for Inorganic Oxidation. <i>Angewandte Chemie</i> , 2017, 129, 5884-5888. | 1.6 | 16 |
| 10672 | An investigation of aromaticity in hydroxybenzenes based on the study of magnetically induced current density. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25382. | 1.0 | 6 |
| 10673 | Structure, Stability, and (Non)Reactivity of the Low-Index Surfaces of Crystalline B ₂ O ₃ . <i>Journal of Physical Chemistry C</i> , 2017, 121, 11346-11354. | 1.5 | 10 |
| 10674 | Computational analysis of site differences in selective aliphatic C-H hydroxylation by nonheme iron-oxo complexes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13924-13930. | 1.3 | 2 |
| 10675 | Kohn-Sham density functional theory calculations of non-resonant and resonant x-ray emission spectroscopy. <i>Journal of Chemical Physics</i> , 2017, 146, . | 1.2 | 29 |
| 10676 | Molecular simulation of liquid crystal sensor based on competitive inclusion effect. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2017, 87, 95-103. | 0.9 | 4 |
| 10677 | Spectroscopic, Structural, and Kinetic Investigation of the Ultrafast Spin Crossover in an Unusual Cobalt(II) Semiquinonate Radical Complex. <i>Chemistry - A European Journal</i> , 2017, 23, 2119-2132. | 1.7 | 36 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10678 | Hydroxo-bridged diiron(Fe^{II}) and dimanganese(Mn^{II}) bisporphyrins: modulation of metal spins by counter anions. Dalton Transactions, 2017, 46, 1012-1037. | 1.6 | 36 |
| 10679 | Utility of extrinsic [60] fullerenes as work function type sensors for amphetamine drug detection: DFT studies. Vacuum, 2017, 136, 156-162. | 1.6 | 123 |
| 10680 | Defect-induced selective oxidation of graphene: A first-principles study. Applied Surface Science, 2017, 396, 243-248. | 3.1 | 4 |
| 10681 | The effects of fluorine substitution on the chemical properties and inhibitory capacity of Donepezil anti-Alzheimer drug; density functional theory and molecular docking calculations. Journal of Molecular Graphics and Modelling, 2017, 71, 124-134. | 1.3 | 10 |
| 10682 | Intermolecular interactions in the solid state structures of neutral and N-protonated 5-alkoxymethyl-8-hydroxyquinolines. Journal of Molecular Structure, 2017, 1133, 307-319. | 1.8 | 3 |
| 10683 | Accurate Intermolecular Potential for the C_{60} Dimer: The Performance of Different Levels of Quantum Theory. Journal of Chemical Theory and Computation, 2017, 13, 274-285. | 2.3 | 20 |
| 10684 | Supramolecular organization of perfluorinated 1H-indazoles in the solid state using X-ray crystallography, SSNMR and sensitive (VCD) and non sensitive (MIR, FIR and Raman) to chirality vibrational spectroscopies. Physical Chemistry Chemical Physics, 2017, 19, 1632-1643. | 1.3 | 18 |
| 10685 | Single-Molecule Conductance Studies of Organometallic Complexes Bearing π -Thienyl Contacting Groups. Chemistry - A European Journal, 2017, 23, 2133-2143. | 1.7 | 50 |
| 10686 | Conformational Analysis and Absolute Configuration of Axially Chiral 1-Aryl and 1,3-Bisaryl-xanthenes. Journal of Organic Chemistry, 2017, 82, 6874-6885. | 1.7 | 14 |
| 10687 | An Ab Initio Exciton Model Including Charge-Transfer Excited States. Journal of Chemical Theory and Computation, 2017, 13, 3493-3504. | 2.3 | 85 |
| 10688 | Structure and hydrophilicity of azo-dye-derived rotaxane: density functional theory approach. Coloration Technology, 2017, 133, 382-390. | 0.7 | 1 |
| 10689 | Photofragmentation of Tetranitromethane: Spin-Unrestricted Time-Dependent Excited-State Molecular Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 3185-3192. | 2.1 | 21 |
| 10690 | Group additivity-Pourbaix diagrams advocate thermodynamically stable nanoscale clusters in aqueous environments. Nature Communications, 2017, 8, 15852. | 5.8 | 27 |
| 10691 | Revisiting the thermochemistry of chlorine fluorides. Journal of Computational Chemistry, 2017, 38, 1930-1940. | 1.5 | 1 |
| 10692 | Mechanistic Studies on Pd(MPAA)-Catalyzed Enantioselective $\text{C}=\text{H}$ Activation Reactions. Springer Theses, 2017, , 83-110. | 0.0 | 0 |
| 10693 | Structural and electronic features of triphenylstibine-functionalized Fischer carbene complexes of molybdenum(0). Polyhedron, 2017, 133, 307-318. | 1.0 | 10 |
| 10694 | Magnetorefrigeration capability of a gadolinium(III) coordination polymer containing trimesic acid: a correlation between the isothermal magnetic entropy change and the gadolinium content. RSC Advances, 2017, 7, 30763-30769. | 1.7 | 6 |
| 10695 | Predicting electronic structure properties of transition metal complexes with neural networks. Chemical Science, 2017, 8, 5137-5152. | 3.7 | 152 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10696 | Evaluation of electronic polarization energy in oligoacene molecular crystals using the solvated supermolecular approach. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 14453-14461. | 1.3 | 7 |
| 10697 | Origin of the Base-Dependent Facial Selectivity in Annulation Reactions of Nazarov-Type Reagents with Unsaturated Indolo[2,3- <i>a</i>]quinolizidine Lactams. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 3969-3979. | 1.2 | 5 |
| 10698 | trans-cis Pd-C rearrangement in hemichelates. <i>Dalton Transactions</i> , 2017, 46, 8125-8137. | 1.6 | 9 |
| 10699 | Orthogonal smectic and nematic ordering in three-ring polar bent-core molecules with anti-parallel arrangement. <i>New Journal of Chemistry</i> , 2017, 41, 5403-5411. | 1.4 | 20 |
| 10700 | Spectroscopic, structural and drug docking studies of carbocysteine. <i>Journal of Molecular Structure</i> , 2017, 1144, 432-442. | 1.8 | 2 |
| 10701 | Quantum Chemical Spin Densities for Radical Cations of Photosynthetic Pigment Models. <i>Photochemistry and Photobiology</i> , 2017, 93, 815-833. | 1.3 | 9 |
| 10702 | Synthesis of Benzodihydrofurans by Asymmetric C-H Insertion Reactions of Donor/Donor Rhodium Carbenes. <i>Chemistry - A European Journal</i> , 2017, 23, 11843-11855. | 1.7 | 43 |
| 10703 | Spectroscopic Observation of the Triplet Diradical State of a Cyclobutadiene. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 10183-10187. | 7.2 | 33 |
| 10704 | Salts Influence Catechins and Flavonoids Encapsulation in Liposomes: A Molecular Dynamics Investigation. <i>Molecular Informatics</i> , 2017, 36, 1700059. | 1.4 | 22 |
| 10705 | Charge-Shift Corrected Electronegativities and the Effect of Bond Polarity and Substituents on Covalent-Ionic Resonance Energy. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5190-5195. | 1.1 | 10 |
| 10706 | Basic Phosphonium Ionic Liquids as Wittig Reagents. <i>ACS Omega</i> , 2017, 2, 2901-2911. | 1.6 | 13 |
| 10707 | Accurate excitation energies of molecules and oligomers from a semilocal density functional. <i>Journal of Chemical Physics</i> , 2017, 146, 234102. | 1.2 | 11 |
| 10708 | Modeling hydroxylated nanosilica: Testing the performance of ReaxFF and FFSiOH force fields. <i>Journal of Chemical Physics</i> , 2017, 146, 224704. | 1.2 | 12 |
| 10709 | Optimization and transferability of non-electrostatic repulsion in the polarizable density embedding model. <i>Journal of Computational Chemistry</i> , 2017, 38, 2108-2117. | 1.5 | 4 |
| 10710 | Relativistic Approximations to Paramagnetic NMR Chemical Shift and Shielding Anisotropy in Transition Metal Systems. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3731-3745. | 2.3 | 26 |
| 10711 | Selectivity of aliphatic alcohols by host-guest chemistry. <i>CrystEngComm</i> , 2017, 19, 3682-3688. | 1.3 | 4 |
| 10712 | Reaction of 8-chloro-5,7-dinitroquinoline with β^2 -dicarbonyl compounds. <i>Russian Journal of Organic Chemistry</i> , 2017, 53, 557-561. | 0.3 | 1 |
| 10713 | (Electro)chemical Oxidation of 6,13-Bis[tri(isopropyl)silylethynyl]pentacene to its Radical Cation and Dication. <i>ChemPhysChem</i> , 2017, 18, 2266-2278. | 1.0 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10714 | Ruthenium(II) Bipyridyl Complexes with Cyclometalated NHC Ligands. <i>Inorganic Chemistry</i> , 2017, 56, 7217-7229. | 1.9 | 33 |
| 10715 | DFT Studies of Ru-Catalyzed C=O versus C-H Bond Functionalization of Aryl Ethers with Organoboronates. <i>Organometallics</i> , 2017, 36, 2354-2363. | 1.1 | 20 |
| 10716 | Reduction of carbon dioxide and organic carbonyls by hydrosilanes catalysed by the perrhenate anion. <i>Catalysis Science and Technology</i> , 2017, 7, 2838-2845. | 2.1 | 42 |
| 10717 | 4,5-Substituted C [∧] C* cyclometalated thiazol-2-ylidene platinum(ii) complexes – synthesis and photophysical properties. <i>Dalton Transactions</i> , 2017, 46, 7800-7812. | 1.6 | 13 |
| 10718 | On the spectral properties of methyl and methoxy derivatives of 1,3-diphenyl-1 H-pyrazolo[3,4-b]quinoxalines: Experiment and DFT/TDDFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 186, 89-98. | 2.0 | 9 |
| 10719 | Conventional and Explicitly Correlated ab Initio Benchmark Study on Water Clusters: Revision of the BEGDB and WATER27 Data Sets. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3136-3152. | 2.3 | 81 |
| 10720 | Internal abstraction of dynemicin A: An MD approach. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 74, 251-264. | 1.3 | 6 |
| 10721 | Can Baird's and Clar's Rules Combined Explain Triplet State Energies of Polycyclic Conjugated Hydrocarbons with Fused 4n and (4n + 2)π-Rings?. <i>Journal of Organic Chemistry</i> , 2017, 82, 6327-6340. | 1.7 | 55 |
| 10722 | para-Azaquinodimethane: A Compact Quinodimethane Variant as an Ambient Stable Building Block for High-Performance Low Band Gap Polymers. <i>Journal of the American Chemical Society</i> , 2017, 139, 8355-8363. | 6.6 | 65 |
| 10723 | DFT insight on oxygen adsorbed platinum trimer cluster (Pt ₃) for CO oxidation. <i>Computational and Theoretical Chemistry</i> , 2017, 1114, 1-7. | 1.1 | 11 |
| 10724 | Halogen atom transfer mechanism of iron-catalyzed direct arylation to form biaryl using Density Functional Theory calculations. <i>Journal of Organometallic Chemistry</i> , 2017, 844, 8-15. | 0.8 | 7 |
| 10725 | Covalent Co-O and Sb-N Bonds Enable Polyoxovanadate Charge Control. <i>Inorganic Chemistry</i> , 2017, 56, 7120-7126. | 1.9 | 15 |
| 10726 | Evaluating the friction of rotary joints in molecular machines. <i>Molecular Systems Design and Engineering</i> , 2017, 2, 235-252. | 1.7 | 9 |
| 10727 | Quantum chemical study on phenethylamines reveals new cation structures. <i>Computational and Theoretical Chemistry</i> , 2017, 1114, 47-54. | 1.1 | 4 |
| 10728 | A theoretical study on the palladium-catalyzed oxidative carbocyclization-alkoxycarbonylation of bisallenes to construct seven-membered carbocycles assisted by olefins. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 5055-5061. | 1.5 | 15 |
| 10729 | Synthesis, Solid State Structure, and Bonding Analysis of a Homoleptic Beryllium Azide. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 8559-8563. | 7.2 | 27 |
| 10730 | Synthesis, structural and biological studies of two new Co(III) complexes with tridentate hydrazone ligand derived from the antihypertensive drug hydralazine. <i>Inorganica Chimica Acta</i> , 2017, 466, 16-29. | 1.2 | 19 |
| 10731 | Theoretical study of hydrogen adsorption in Ti-decorated capped carbon nanotube. <i>Molecular Physics</i> , 2017, 115, 2515-2520. | 0.8 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10732 | Arylthio- and Arylseleno-Substituted <i>s</i> -Heptazines. <i>Chemistry - A European Journal</i> , 2017, 23, 12510-12518. | 1.7 | 12 |
| 10733 | On the applicability of density functional theory to manganese-based complexes with catalytic activity toward water oxidation. <i>Journal of Computational Chemistry</i> , 2017, 38, 1747-1751. | 1.5 | 3 |
| 10734 | Comparative study of semilocal density functionals on solids and surfaces. <i>Chemical Physics Letters</i> , 2017, 682, 38-42. | 1.2 | 12 |
| 10735 | Kinetics and branching fractions of the hydrogen abstraction reaction from methyl butenoates by H atoms. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 16563-16575. | 1.3 | 29 |
| 10736 | Silver(III)-Silver(III) Interactions that Stabilize the <i>syn</i> Form in a Porphyrin Dimer Upon Oxidation. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 8849-8854. | 7.2 | 33 |
| 10737 | Turn on-fluorescence response of monomethine cyanines caused by noncovalent binding to ct-DNA. <i>Dyes and Pigments</i> , 2017, 145, 202-207. | 2.0 | 6 |
| 10738 | Improved <i>K_a</i> Prediction of Substituted Alcohols, Phenols, and Hydroperoxides in Aqueous Medium Using Density Functional Theory and a Cluster-Continuum Solvation Model. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4698-4706. | 1.1 | 77 |
| 10739 | Real-time monitoring of hydrophobic aggregation reveals a critical role of cooperativity in hydrophobic effect. <i>Nature Communications</i> , 2017, 8, 15639. | 5.8 | 67 |
| 10740 | A theoretical study on the mechanism of ruthenium(<i>ii</i>)-catalyzed phosphoryl-directed <i>ortho</i> -selective C-H bond activations: the phosphoryl hydroxy group triggered Ru(<i>ii</i>)/Ru(0) catalytic cycle. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1482-1492. | 2.3 | 14 |
| 10741 | A photoinduced reaction of perfluoroalkyl halides with 1,3-diarylprop-2-yn-1-ones catalyzed by DABSO. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1745-1750. | 2.3 | 21 |
| 10742 | <i>Alkenyl</i> tyrosines Accessed by Suzuki-Miyaura Coupling: A Key Intermediate in the Synthesis and Mechanistic Study of Povarov Multicomponent Reactions. <i>Asian Journal of Organic Chemistry</i> , 2017, 6, 913-920. | 1.3 | 7 |
| 10743 | Dithiafulvenyl-Extended <i>N</i> -Heterotriangulenes and Their Interaction with C ₆₀ : Cooperative Fluorescence. <i>Chemistry - A European Journal</i> , 2017, 23, 12353-12362. | 1.7 | 8 |
| 10744 | Are Electron Affinity and Ionization Potential Intrinsic Parameters to Predict the Electron or Hole Acceptor Character of Amorphous Molecular Materials?. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2445-2449. | 2.1 | 40 |
| 10745 | Mechanistic study on ligand-controlled copper-catalyzed regiodivergent silacarboxylation of allenes with carbon dioxide and silylborane. <i>RSC Advances</i> , 2017, 7, 29035-29041. | 1.7 | 10 |
| 10746 | Polarizable and Non-Polarizable Force Field Representations of Ferric Cation and Validations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5718-5729. | 1.2 | 7 |
| 10747 | Substantial Intramolecular Charge Transfer Induces Long Emission Wavelengths and Mega Stokes Shifts in 6-Aminocoumarins. <i>Journal of Physical Chemistry C</i> , 2017, 121, 13274-13279. | 1.5 | 55 |
| 10748 | The Origins of Dramatic Differences in Five-Membered vs Six-Membered Chelation of Pd(II) on Efficiency of C(sp ³)-H Bond Activation. <i>Journal of the American Chemical Society</i> , 2017, 139, 8514-8521. | 6.6 | 96 |
| 10749 | 1,2-Diaza-4-phosphaferrocenes: synthesis, structural characterization, ⁵⁷ Fe Mössbauer spectrum analysis, and DFT calculation. <i>Dalton Transactions</i> , 2017, 46, 8354-8358. | 1.6 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10750 | Reduced graphene oxide-catalyzed oxidative coupling reaction of 4-methoxyphenol in aerobic aqueous solution. <i>Carbon</i> , 2017, 121, 418-425. | 5.4 | 18 |
| 10751 | Copper ion interaction with the RNase catalytic site fragment of the angiogenin protein: an experimental and theoretical investigation. <i>Dalton Transactions</i> , 2017, 46, 8524-8538. | 1.6 | 6 |
| 10752 | Synthesis and fluorosolvatochromic properties of 1,7-annulated indoles. <i>New Journal of Chemistry</i> , 2017, 41, 7331-7338. | 1.4 | 5 |
| 10753 | Functionalised metal-organic frameworks: a novel approach to stabilising single metal atoms. <i>Journal of Materials Chemistry A</i> , 2017, 5, 15559-15566. | 5.2 | 24 |
| 10754 | A Quantum-mechanical Study of the Binding Pocket of Proteorhodopsin: Absorption and Vibrational Spectra Modulated by Analogue Chromophores. <i>Photochemistry and Photobiology</i> , 2017, 93, 1399-1406. | 1.3 | 7 |
| 10755 | 1D Energetic Metal-Organic Framework: Sodium 6-Nitro-5-oxidopyrazolo[3,4-c][1,2,5]oxadiazol-4-ide with Good Thermal Stability. <i>ChemistrySelect</i> , 2017, 2, 4673-4677. | 0.7 | 10 |
| 10756 | Exploring the substrate selectivity of human sEH and M. tuberculosis EHB using QM/MM. <i>Structural Chemistry</i> , 2017, 28, 1501-1511. | 1.0 | 9 |
| 10757 | Can DFT and ab initio methods adequately describe binding energies in strongly interacting C ₆ X ₆ -C ₂ X ₂ complexes?. <i>Chemical Physics</i> , 2017, 493, 12-19. | 0.9 | 7 |
| 10758 | Propane CH activation by palladium complexes bearing ligands with Charge-shift bonding characteristics: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2017, 1115, 30-36. | 1.1 | 7 |
| 10759 | Synthesis, DSC, Vis spectroscopy and DFT/DFT calculations on 6-substituted halogen derivatives of 1,3-diphenyl-1H-pyrazolo[3,4-c][1,2,5]oxadiazol-4-ide. <i>Journal of Molecular Structure</i> , 2017, 1146, 554-561. | 1.5 | 13 |
| 10760 | Valence Bond Theory Reveals Hidden Delocalized Diradical Character of Polyenes. <i>Journal of the American Chemical Society</i> , 2017, 139, 9302-9316. | 6.6 | 33 |
| 10761 | Self-consistent hybrid functionals for solids: a fully-automated implementation. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 314001. | 0.7 | 23 |
| 10762 | Dimension reduction in conformational analysis: a two-rotor mathematical model of amino acid diamide conformational potential energy surface. <i>Canadian Journal of Chemistry</i> , 2017, 95, 830-836. | 0.6 | 2 |
| 10763 | Silver(III) Interactions that Stabilize the <i>syn</i> Form in a Porphyrin Dimer Upon Oxidation. <i>Angewandte Chemie</i> , 2017, 129, 8975-8980. | 1.6 | 8 |
| 10764 | Structures and photophysical properties of 3,4-diaryl-1H-pyrrol-2,5-diimines and 2,3-diarylmaleimides. <i>Journal of Molecular Structure</i> , 2017, 1146, 554-561. | 1.8 | 12 |
| 10765 | On the feasibility of reactions through the fullerene wall: a theoretical study of NH _x @C ₆₀ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17199-17209. | 1.3 | 4 |
| 10766 | Quantum Chemical Mass Spectrometry: Verification and Extension of the Mobile Proton Model for Histidine. <i>Journal of the American Society for Mass Spectrometry</i> , 2017, 28, 1227-1235. | 1.2 | 16 |
| 10767 | Dimeric nature of N-coordinated Mg and Ca ions in metalloorganic compounds. The topological analysis of ELF functions for Mg and Ca bonds. <i>Polyhedron</i> , 2017, 129, 22-29. | 1.0 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10768 | Comparison of metal-binding strength between methionine and cysteine residues: Implications for the design of metal-binding motifs in proteins. <i>Biophysical Chemistry</i> , 2017, 224, 32-39. | 1.5 | 16 |
| 10769 | Operando Solid-State NMR Observation of Solvent-Mediated Adsorption-Reaction of Carbohydrates in Zeolites. <i>ACS Catalysis</i> , 2017, 7, 3489-3500. | 5.5 | 70 |
| 10770 | The mechanism of the Ser-(cis)Ser-Lys catalytic triad of peptide amidases. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12343-12354. | 1.3 | 17 |
| 10771 | Croconato-bridged copper(II) complexes: synthesis, structure and magnetic characterization. <i>New Journal of Chemistry</i> , 2017, 41, 3846-3856. | 1.4 | 5 |
| 10772 | Structure of aryl O-demethylase offers molecular insight into a catalytic tyrosine-dependent mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E3205-E3214. | 3.3 | 24 |
| 10773 | Synthesis, spectroscopic characterization, X-ray structure and DFT calculations of Ni(II)bis(3,4) Tj ETQq1 1 0.784314 rgBT /Oylock 10 0.6 | 0.6 | 3 |
| 10774 | Resolution of isomeric new designer stimulants using gas chromatography – Vacuum ultraviolet spectroscopy and theoretical computations. <i>Analytica Chimica Acta</i> , 2017, 971, 55-67. | 2.6 | 67 |
| 10775 | Computing sextic centrifugal distortion constants by DFT: A benchmark analysis on halogenated compounds. <i>Journal of Molecular Spectroscopy</i> , 2017, 335, 117-125. | 0.4 | 24 |
| 10776 | Physical Molecular Mechanics Method for Damped Dispersion. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2855-2862. | 1.1 | 12 |
| 10777 | Theoretical analysis of electrochromism under redox of bis(3-thienyl)/(2-thienyl)hexafluorocyclopentene: effects of charged and substituted systems. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 9281-9291. | 1.3 | 3 |
| 10778 | Effects of the locality of a potential derived from hybrid density functionals on Kohn–Sham orbitals and excited states. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10177-10186. | 1.3 | 14 |
| 10779 | A tunable and sizable bandgap of a g-C ₃ N ₄ /graphene/g-C ₃ N ₄ sandwich heterostructure: a van der Waals density functional study. <i>Journal of Materials Chemistry C</i> , 2017, 5, 3830-3837. | 2.7 | 86 |
| 10780 | Understanding how cAMP-dependent protein kinase can catalyze phosphoryl transfer in the presence of Ca ²⁺ and Sr ²⁺ : a QM/MM study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10377-10394. | 1.3 | 6 |
| 10781 | A computational study of the Diels-Alder reactions between 2,3-dibromo-1,3-butadiene and maleic anhydride. <i>Chemical Physics Letters</i> , 2017, 683, 598-605. | 1.2 | 13 |
| 10782 | Synthesis, Spectroelectrochemical Behavior, and Chiroptical Switching of Tris(η ² -diketonato) Complexes of Ruthenium(III), Chromium(III), and Cobalt(III). <i>Inorganic Chemistry</i> , 2017, 56, 4555-4567. | 1.9 | 18 |
| 10783 | Spectroscopic and Computational Studies of Spin States of Iron(IV) Nitrido and Imido Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 4751-4768. | 1.9 | 41 |
| 10784 | Precise through-space control of an abiotic electrophilic aromatic substitution reaction. <i>Nature Communications</i> , 2017, 8, 14840. | 5.8 | 13 |
| 10785 | Composition-directed Fe _X Mo ₂ X ₂ P bimetallic catalysts for hydrodeoxygenation reactions. <i>Catalysis Science and Technology</i> , 2017, 7, 1857-1867. | 2.1 | 48 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10804 | Investigating cyclic sotolon, maple furanone and their dimers in solution using optical rotation, electronic circular dichroism and vibrational circular dichroism. <i>Tetrahedron</i> , 2017, 73, 2432-2438. | 1.0 | 5 |
| 10805 | A novel role for methyl cysteinylglycine, a cysteine derivative, in cesium accumulation in <i>Arabidopsis thaliana</i> . <i>Scientific Reports</i> , 2017, 7, 43170. | 1.6 | 15 |
| 10806 | Theoretical Studies of the Electronic Absorption Spectra of Thiamin Diphosphate in Pyruvate Decarboxylase. <i>Biochemistry</i> , 2017, 56, 1854-1864. | 1.2 | 10 |
| 10807 | N ₂ O Formation via Reductive Disproportionation of NO by Mononuclear Copper Complexes: A Mechanistic DFT Study. <i>Inorganic Chemistry</i> , 2017, 56, 3820-3833. | 1.9 | 25 |
| 10808 | in/out Isomerism of cyclophanes: a theoretical account of 2,6,15-trithia-[34,10][7]metacyclophane and [34,10][7]metacyclophane as well as their halogen substituted analogues. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 9500-9508. | 1.3 | 3 |
| 10809 | The assembly of S ₃ N ⁴ ligands decorated with an azo-dye as potential sensors for heavy metal ions. <i>Dalton Transactions</i> , 2017, 46, 5229-5239. | 1.6 | 7 |
| 10810 | Hydrogenation and Deuteration of C ₂ H ₂ and C ₂ H ₄ on Cold Grains: A Clue to the Formation Mechanism of C ₂ H ₆ with Astronomical Interest. <i>Astrophysical Journal</i> , 2017, 837, 155. | 1.6 | 26 |
| 10811 | Femtosecond stimulated Raman study of the photoactive flavoprotein AppABLUf. <i>Chemical Physics Letters</i> , 2017, 683, 365-369. | 1.2 | 14 |
| 10812 | Synthesis and properties of a trapezoid shaped macrocycle with different [n]yne units. <i>RSC Advances</i> , 2017, 7, 17117-17121. | 1.7 | 4 |
| 10813 | Role of exact exchange in thermally-assisted-occupation density functional theory: A proposal of new hybrid schemes. <i>Journal of Chemical Physics</i> , 2017, 146, 044102. | 1.2 | 38 |
| 10814 | Covalent Metal-Metal-Bonded Mn ₄ Tetrahedron Inscribed within a Four-Coordinate Manganese Cubane Cluster, As Evidenced by Unexpected Temperature-Independent Diamagnetism. <i>Inorganic Chemistry</i> , 2017, 56, 3733-3737. | 1.9 | 5 |
| 10815 | Semilocal exchange hole with an application to range-separated density functionals. <i>Physical Review B</i> , 2017, 95, . | 1.1 | 19 |
| 10816 | Embedded and DFT Calculations on the Crystal Structures of Small Alkanes, Notably Propane. <i>Crystal Growth and Design</i> , 2017, 17, 1636-1646. | 1.4 | 18 |
| 10817 | Assembly Mechanism of Zr-Containing and Other TM-Containing Polyoxometalates. <i>Inorganic Chemistry</i> , 2017, 56, 4148-4156. | 1.9 | 15 |
| 10818 | Dinuclear Rhenium Complex with a Proton Responsive Ligand as a Redox Catalyst for the Electrochemical CO ₂ Reduction. <i>Inorganic Chemistry</i> , 2017, 56, 4176-4185. | 1.9 | 50 |
| 10819 | Ab Initio Studies on the Clathrate Hydrates of Some Nitrogen- and Sulfur-Containing Gases. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2620-2626. | 1.1 | 16 |
| 10820 | Photoswitching of azobenzene-containing self-assembled monolayers as a tool for control over silicon surface electronic properties. <i>Journal of Chemical Physics</i> , 2017, 146, 104703. | 1.2 | 15 |
| 10821 | First Evidence of Polymorphism in Furosemide Solvates. <i>Crystal Growth and Design</i> , 2017, 17, 2333-2341. | 1.4 | 17 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10822 | CO oxidation by the atomic oxygen on silver clusters: structurally dependent mechanisms generating free or chemically bonded CO ₂ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 196-203. | 1.3 | 22 |
| 10823 | Large Magnetic Anisotropy in Linear CollComplexes - Ab Initio Investigation of the Roles of Ligand Field, Structural Distortion, and Conformational Dynamics. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 659-668. | 1.0 | 9 |
| 10824 | Bacteriochlorins with a Twist: Discovery of a Unique Mechanism to Red-Shift the Optical Spectra of Bacteriochlorins. <i>Journal of the American Chemical Society</i> , 2017, 139, 548-560. | 6.6 | 32 |
| 10825 | First-Principles Study of Pressure-Induced Phase Transition in CuGaO ₂ . <i>Brazilian Journal of Physics</i> , 2017, 47, 42-45. | 0.7 | 0 |
| 10826 | Understanding the insight into the mechanisms and dynamics of the Cl-initiated oxidation of (CH ₃) ₃ CC(O)X and the subsequent reactions in the presence of NO and O ₂ (X = F, Cl, and Br). <i>Chemosphere</i> , 2017, 171, 49-56. | 4.2 | 6 |
| 10827 | Ruthenium(II) DMSO complexes with C ⁺ * cyclometalated phenylimidazol NHC ligands. <i>Journal of Organometallic Chemistry</i> , 2017, 829, 101-107. | 0.8 | 12 |
| 10828 | Theoretical Modeling of Vibrational Spectra in the Liquid Phase. <i>Springer Theses</i> , 2017, , . | 0.0 | 8 |
| 10829 | Systematic investigation of the excited-state properties of anthracene-dicarboxylic acids. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 337, 207-215. | 2.0 | 17 |
| 10830 | Sensitive and Accurate ¹³ C Kinetic Isotope Effect Measurements Enabled by Polarization Transfer. <i>Journal of the American Chemical Society</i> , 2017, 139, 43-46. | 6.6 | 50 |
| 10831 | Validating a Density Functional Theory Approach for Predicting the Redox Potentials Associated with Charge Carriers and Excitons in Polymeric Photocatalysts. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1498-1506. | 1.5 | 40 |
| 10832 | Kinetic enantioselectivity of a protonated bis(diamido)-bridged basket resorcin[4]arene towards alanine peptides. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 1183-1189. | 1.5 | 3 |
| 10833 | Integrating ion mobility spectrometry into mass spectrometry-based exposome measurements: what can it add and how far can it go?. <i>Bioanalysis</i> , 2017, 9, 81-98. | 0.6 | 66 |
| 10834 | A DFT study on the structure–reactivity relationship of aliphatic oxime derivatives as copper chelating agents and malachite flotation collectors. <i>Journal of Industrial and Engineering Chemistry</i> , 2017, 46, 404-415. | 2.9 | 53 |
| 10835 | Efficient Constrained Density Functional Theory Implementation for Simulation of Condensed Phase Electron Transfer Reactions. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 587-601. | 2.3 | 40 |
| 10836 | Identification of Second Shell Coordination in Transition Metal Species Using Theoretical XANES: Example of Ti–(C, Si, Ge) Complexes. <i>Journal of Physical Chemistry A</i> , 2017, 121, 162-167. | 1.1 | 7 |
| 10837 | Vacuum-Evaporable Spin-Crossover Complexes in Direct Contact with a Solid Surface: Bismuth versus Gold. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1210-1219. | 1.5 | 71 |
| 10838 | Highly accurate benchmark calculations of the interaction energies in the complexes C ₆ H ₆ ·Á·Á·C ₆ H ₆ X ₆ (X = F, Cl, Br, and I). <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25345. | | 24 |
| 10839 | Solvent free, palladium catalyzed highly facile synthesis of diaryl disulfides from aryl thiols. <i>Tetrahedron Letters</i> , 2017, 58, 527-530. | 0.7 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10840 | Directing Energy Transfer in Panchromatic Platinum Complexes for Dual Visâ€“Near-IR or Dual Visible Emission from Ij-Bonded BODIPY Dyes. <i>Inorganic Chemistry</i> , 2017, 56, 914-930. | 1.9 | 13 |
| 10841 | Magnetic coupling and relaxation in Fe[N(SiPh2Me)2]2 molecular magnet. <i>Structural Chemistry</i> , 2017, 28, 975-983. | 1.0 | 4 |
| 10842 | Rapid Method Development in Hydrophilic Interaction Liquid Chromatography for Pharmaceutical Analysis Using a Combination of Quantitative Structureâ€“Retention Relationships and Design of Experiments. <i>Analytical Chemistry</i> , 2017, 89, 1870-1878. | 3.2 | 41 |
| 10843 | Total Facial Discrimination of 1,3-Dipolar Cycloadditions in a ^d-Erythrose 1,3-Dioxane Template: Computational Studies of a Concerted Mechanism. <i>Journal of Organic Chemistry</i> , 2017, 82, 982-991. | 1.7 | 6 |
| 10844 | Enhancing the conductivity of molecular electronic devices. <i>Journal of Chemical Physics</i> , 2017, 146, . | 1.2 | 39 |
| 10845 | Rational design of model Pd(ⁱⁱ)-catalysts for Câ€“H activation involving ligands with charge-shift bonding characteristics. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2417-2424. | 1.3 | 8 |
| 10846 | A Theoretical Investigation of the Structure and Optical Properties of a Silver Cluster in Solid Form and in Solution. <i>Journal of Physical Chemistry A</i> , 2017, 121, 326-333. | 1.1 | 7 |
| 10847 | The Solvation Structure of Lithium Ions in an Ether Based Electrolyte Solution from First-Principles Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2017, 121, 180-188. | 1.2 | 41 |
| 10848 | Effect of ionic charge on O<math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mtext /></mml:mrow></math>Hâ€“Se hydrogen bond: A computational study. <i>Computational and Theoretical Chemistry</i> , 2017, 1102, 127-138. | 1.1 | 13 |
| 10849 | Anticancer, antimicrobial, spectral, voltammetric and DFT studies with Cu(II) complexes of 2-hydroxy-5-methoxyacetophenone thiosemicarbazone and its N(4)- substituted derivatives. <i>Journal of Organometallic Chemistry</i> , 2017, 831, 23-35. | 0.8 | 31 |
| 10850 | HLE16: A Local Kohnâ€“Sham Gradient Approximation with Good Performance for Semiconductor Band Gaps and Molecular Excitation Energies. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 380-387. | 2.1 | 78 |
| 10851 | A theoretical study of the diastereoselective allylation of aldehydes with new chiral allylsilanes. <i>Journal of Molecular Modeling</i> , 2017, 23, 5. | 0.8 | 17 |
| 10852 | Accurate Dissociation of Chemical Bonds Using DFT-in-DFT Embedding Theory with External Orbital Orthogonality. <i>Journal of Physical Chemistry A</i> , 2017, 121, 256-264. | 1.1 | 24 |
| 10853 | Large pi-systems containing Wâ€“N=Nâ€“W groups. <i>Canadian Journal of Chemistry</i> , 2017, 95, 214-221. | 0.6 | 0 |
| 10854 | Hypoelectronicity and Chirality in Dimetallaboranes of Group 9 Metals. <i>Inorganic Chemistry</i> , 2017, 56, 351-358. | 1.9 | 1 |
| 10855 | The influence of halides in polyoxotitanate cages; dipole moment, splitting and expansion of d-orbitals and electronâ€“electron repulsion. <i>Dalton Transactions</i> , 2017, 46, 578-585. | 1.6 | 17 |
| 10856 | Multidentate 2-pyridyl-phosphine ligands â€“ towards ligand tuning and chirality. <i>Dalton Transactions</i> , 2017, 46, 814-824. | 1.6 | 14 |
| 10857 | Frozen Virtual Natural Orbitals for Coupled-Cluster Linear-Response Theory. <i>Journal of Physical Chemistry A</i> , 2017, 121, 708-716. | 1.1 | 40 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10858 | Divergent reactivity of a new dinuclear xanthene-bridged bis(iminopyridine) di-nickel complex with alkynes. Dalton Transactions, 2017, 46, 5605-5616. | 1.6 | 29 |
| 10859 | Assessment of Interstate Spin-Orbit Couplings from Linear Response Amplitudes. Journal of Chemical Theory and Computation, 2017, 13, 749-766. | 2.3 | 18 |
| 10860 | Carbamohydrazone thioate derivative—experimental and theoretical explorations of the crystal and molecular structure. Structural Chemistry, 2017, 28, 801-812. | 1.0 | 1 |
| 10861 | Compounds based on 3-amino-4-(5-methyl-1,2,4-oxadiazol-3-yl)furazan as insensitive energetic materials. New Journal of Chemistry, 2017, 41, 1202-1211. | 1.4 | 27 |
| 10862 | <i>mer</i> , <i>fac</i> , and Bidentate Coordination of an Alkyl-POP Ligand in the Chemistry of Nonclassical Osmium Hydrides. Inorganic Chemistry, 2017, 56, 676-683. | 1.9 | 29 |
| 10863 | Density Functional Theory Investigation of Possible Structures of Radicals in Coal Undergoing O ₂ Chemisorption at Ambient Temperature. Energy & Fuels, 2017, 31, 953-958. | 2.5 | 20 |
| 10864 | Hamiltonian Matrix Correction Based Density Functional Valence Bond Method. Journal of Chemical Theory and Computation, 2017, 13, 627-634. | 2.3 | 18 |
| 10865 | Understanding dispersive charge-transport in crystalline organic-semiconductors. Physical Chemistry Chemical Physics, 2017, 19, 231-236. | 1.3 | 3 |
| 10866 | Radical Reaction Control in the AdoMet Radical Enzyme CDG Synthase (QueE): Consolidate, Destabilize, Accelerate. Chemistry - A European Journal, 2017, 23, 953-962. | 1.7 | 10 |
| 10867 | Quantitative Assessment of Halogen Bonding Utilizing Vibrational Spectroscopy. Inorganic Chemistry, 2017, 56, 488-502. | 1.9 | 91 |
| 10868 | Prediction of retention in hydrophilic interaction liquid chromatography using solute molecular descriptors based on chemical structures. Journal of Chromatography A, 2017, 1486, 59-67. | 1.8 | 47 |
| 10869 | Newly assigned microwave transitions and a global analysis of the combined microwave/millimeter wave rotational spectra of 9-fluorenone and benzophenone. Journal of Molecular Spectroscopy, 2017, 335, 43-48. | 0.4 | 5 |
| 10870 | Density functional theory for modelling large molecular adsorbate—surface interactions: a mini-review and worked example. Molecular Simulation, 2017, 43, 327-345. | 0.9 | 39 |
| 10871 | Four- and Five-Component Syntheses and Photophysical Properties of Emission Solvatochromic 3-Aminovinylquinoxalines. Journal of Organic Chemistry, 2017, 82, 567-578. | 1.7 | 32 |
| 10872 | Photoabsorption Tolerance of Intrinsic Point Defects and Oxidation in Black Phosphorus Quantum Dots. Journal of Physical Chemistry Letters, 2017, 8, 161-166. | 2.1 | 21 |
| 10873 | Photochemistry of Coronene in Cosmic Water Ice Analogs at Different Concentrations. Astrophysical Journal, 2017, 848, 112. | 1.6 | 23 |
| 10874 | Efficient and Accurate Born-Oppenheimer Molecular Dynamics for Large Molecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5479-5485. | 2.3 | 16 |
| 10875 | Insights into the origin of the excited transitions in graphene quantum dots interacting with heavy metals in different media. Physical Chemistry Chemical Physics, 2017, 19, 30445-30463. | 1.3 | 29 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10876 | A study of the Group 1 metal tetra-aza macrocyclic complexes [M(Me ₄ cyclen)(L)] ⁺ using electronic structure calculations. Dalton Transactions, 2017, 46, 15301-15310. | 1.6 | 4 |
| 10877 | Unifying Exchange Sensitivity in Transition-Metal Spin-State Ordering and Catalysis through Bond Valence Metrics. Journal of Chemical Theory and Computation, 2017, 13, 5443-5457. | 2.3 | 43 |
| 10878 | A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. Physical Chemistry Chemical Physics, 2017, 19, 32184-32215. | 1.3 | 1,230 |
| 10879 | Exchange-correlation energies of atoms from efficient density functionals: influence of the electron density. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 245004. | 0.6 | 0 |
| 10880 | Raman and Impedance Spectroscopy under Applied Dc Bias Insights on the Electrical Transport for Donor:Acceptor Nanocomposites Based on Poly(vinyl carbazole) and TiO ₂ Quantum Dots. Journal of Physical Chemistry C, 2017, 121, 23383-23391. | 1.5 | 15 |
| 10881 | Exploring the Relation Between Intramolecular Conjugation and Band Dispersion in One-Dimensional Polymers. Journal of Physical Chemistry C, 2017, 121, 27118-27125. | 1.5 | 29 |
| 10882 | Synthesis of <i>N</i> = 8 Armchair Graphene Nanoribbons from Four Distinct Polydiacetylenes. Journal of the American Chemical Society, 2017, 139, 15878-15890. | 6.6 | 78 |
| 10883 | Optical Gaps in Pristine and Heavily Doped Silicon Nanocrystals: DFT versus Quantum Monte Carlo Benchmarks. Journal of Chemical Theory and Computation, 2017, 13, 6061-6067. | 2.3 | 11 |
| 10884 | Vibrational spectroscopic characterization of arylisoquinolines by means of Raman spectroscopy and density functional theory calculations. Physical Chemistry Chemical Physics, 2017, 19, 29918-29926. | 1.3 | 17 |
| 10885 | Aminoquinoline Fluorescent Labels Obstruct Efficient Removal of <i>N</i> -Glycan Core 1 (6) Fucose by Bovine Kidney α -Fucosidase (BKF). Journal of Proteome Research, 2017, 16, 4237-4243. | 1.8 | 16 |
| 10886 | Introducing DDEC6 atomic population analysis: part 3. Comprehensive method to compute bond orders. RSC Advances, 2017, 7, 45552-45581. | 1.7 | 327 |
| 10887 | An investigation of hybridization and the orbital models of molecular electronic structure for CH ₄ , NH ₃ , and H ₂ O. Canadian Journal of Chemistry, 2017, 95, 1314-1322. | 0.6 | 9 |
| 10888 | Singly and Doubly N-Confused Calix[4]phyrin Organoplatinum(II) Complexes as Near-IR Triplet Sensitizers. Inorganic Chemistry, 2017, 56, 12572-12580. | 1.9 | 32 |
| 10889 | Development of a TDDFT-Based Protocol with Local Hybrid Functionals for the Screening of Potential Singlet Fission Chromophores. Journal of Chemical Theory and Computation, 2017, 13, 4984-4996. | 2.3 | 57 |
| 10890 | Nonlinear Optical Properties of the Hula Hoop [n]Cycloparaphenylenes and Their Halo Derivatives at Nd:YAG Laser Frequency. ChemistrySelect, 2017, 2, 8393-8401. | 0.7 | 4 |
| 10891 | Synthesis and Crystal Structure of Solvated Complexes of Copper(II) with Serine and Phenanthroline and Their Solid-State-to-Solid-State Transformation into One Stable Solvate. Crystal Growth and Design, 2017, 17, 6049-6061. | 1.4 | 10 |
| 10892 | A Computational Scheme To Evaluate Hamaker Constants of Molecules with Practical Size and Anisotropy. Journal of Chemical Theory and Computation, 2017, 13, 5217-5230. | 2.3 | 16 |
| 10893 | Speed-Up of the Excited-State Benchmarking: Double-Hybrid Density Functionals as Test Cases. Journal of Chemical Theory and Computation, 2017, 13, 5539-5551. | 2.3 | 33 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10894 | PAMAM Dendrimers as Support for the Synthesis of Gold Nanoparticles: Understanding the Effect of the Terminal Groups. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8124-8135. | 1.1 | 22 |
| 10895 | Role of π -Radicals in the Spin Connectivity of Clusters and Networks of Tb Double-Decker Single Molecule Magnets. <i>ACS Nano</i> , 2017, 11, 10750-10760. | 7.3 | 24 |
| 10896 | Crystal structures and magnetic properties of two series of phenoxo- μ_2 bridged dinuclear Ln ₂ (Ln = Gd, Tb, Dy) complexes. <i>Dalton Transactions</i> , 2017, 46, 16294-16305. | 1.6 | 34 |
| 10897 | Comparative Assessment of Computational Methods for Free Energy Calculations of Ionic Hydration. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2763-2775. | 2.5 | 20 |
| 10898 | Electronically Excited States in Solution via a Smooth Dielectric Model Combined with Equation-of-Motion Coupled Cluster Theory. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5572-5581. | 2.3 | 10 |
| 10899 | Importance of Nonclassical π -Hole Interactions for the Reactivity of μ_3 -Iodane Complexes. <i>Journal of Organic Chemistry</i> , 2017, 82, 11799-11805. | 1.7 | 45 |
| 10900 | Dual-Phase Mechanism for the Catalytic Conversion of <i>n</i> -Butane to Maleic Anhydride by the Vanadyl Pyrophosphate Heterogeneous Catalyst. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24069-24076. | 1.5 | 14 |
| 10901 | Phosphoramidate hydrolysis catalyzed by human histidine triad nucleotide binding protein 1 (hHint1): a cluster-model DFT computational study. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 8661-8668. | 1.5 | 7 |
| 10902 | Quantum Chemical Fragment Precursor Tests: Accelerating de novo annotation of tandem mass spectra. <i>Analytica Chimica Acta</i> , 2017, 995, 52-64. | 2.6 | 11 |
| 10903 | Homoleptic Trivalent Tris(alkyl) Rare Earth Compounds. <i>Journal of the American Chemical Society</i> , 2017, 139, 16862-16874. | 6.6 | 22 |
| 10904 | B(OH) ₄ ⁻ hydration and association in sodium metaborate solutions by X-ray diffraction and empirical potential structure refinement. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27878-27887. | 1.3 | 34 |
| 10905 | Photoreactions of Phenylborylene with Dinitrogen and Carbon Monoxide. <i>Journal of the American Chemical Society</i> , 2017, 139, 15151-15159. | 6.6 | 61 |
| 10906 | Torsional Barriers to Rotation and Planarization in Heterocyclic Oligomers of Value in Organic Electronics. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5624-5638. | 2.3 | 30 |
| 10907 | Evaluation of the Factors Impacting the Accuracy of ¹³ C NMR Chemical Shift Predictions using Density Functional Theory: The Advantage of Long-Range Corrected Functionals. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5798-5819. | 2.3 | 77 |
| 10908 | Quantum Chemical Modeling of Cycloaddition Reaction in a Self-Assembled Capsule. <i>Journal of the American Chemical Society</i> , 2017, 139, 15494-15503. | 6.6 | 35 |
| 10909 | An interesting 1,4,2,5-dioxadiazine-furazan system: structural modification by incorporating versatile functionalities. <i>Dalton Transactions</i> , 2017, 46, 14301-14309. | 1.6 | 17 |
| 10910 | A biphosphinic ruthenium complex with potent anti-bacterial and anti-cancer activity. <i>New Journal of Chemistry</i> , 2017, 41, 13085-13095. | 1.4 | 22 |
| 10911 | Control of C-H Bond Activation by Mo-Oxo Complexes: μ_2 or Bond Dissociation Free Energy (BDFE)? <i>Inorganic Chemistry</i> , 2017, 56, 12319-12327. | 1.9 | 18 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10912 | Theoretical illumination of highly original photoreactive $3d^3$ MC states and the mechanism of the photochemistry of Ru(d^8) tris(bidentate) complexes. Physical Chemistry Chemical Physics, 2017, 19, 27765-27778. | 1.3 | 30 |
| 10913 | A pair of 3D enantiotopic zinc(II) complexes based on two asymmetric achiral ligands. Dalton Transactions, 2017, 46, 14779-14784. | 1.6 | 12 |
| 10914 | Calculating the geometry and Raman spectrum of physiological bis(l-histidinato)copper(II): an assessment of DFT functionals for aqueous and isolated systems. Journal of Molecular Modeling, 2017, 23, 290. | 0.8 | 9 |
| 10915 | Asymmetric Induction in <i>C</i> -Alkylation of Tropane-Derived Enamines: Congruence Between Computation and Experiment. Journal of Organic Chemistry, 2017, 82, 10479-10488. | 1.7 | 9 |
| 10916 | An efficient and durable novel catalyst support with superior electron-donating properties and fuel diffusivity for a direct methanol fuel cell. Catalysis Science and Technology, 2017, 7, 5079-5091. | 2.1 | 19 |
| 10917 | How To Arrive at Accurate Benchmark Values for Transition Metal Compounds: Computation or Experiment?. Journal of Chemical Theory and Computation, 2017, 13, 5291-5316. | 2.3 | 101 |
| 10918 | Theoretical Insight into $C(sp^3)-F$ Bond Activations and Origins of Chemo- and Regioselectivities of σ -Tunable Nickel-Mediated/Catalyzed Couplings of 2-Trifluoromethyl-1-alkenes with Alkynes. Organometallics, 2017, 36, 3739-3749. | 1.1 | 30 |
| 10919 | Solvent water interactions within the active site of the membrane type I matrix metalloproteinase. Physical Chemistry Chemical Physics, 2017, 19, 30316-30331. | 1.3 | 16 |
| 10920 | Persulfate-promoted benzylic mono- and difluorination: A mechanistic study. Computational and Theoretical Chemistry, 2017, 1119, 10-18. | 1.1 | 6 |
| 10921 | Degradation of Carbonyl Hydroperoxides in the Atmosphere and in Combustion. Journal of the American Chemical Society, 2017, 139, 15821-15835. | 6.6 | 34 |
| 10922 | Picosecond sulfur K-edge X-ray absorption spectroscopy with applications to excited state proton transfer. Structural Dynamics, 2017, 4, 044021. | 0.9 | 15 |
| 10923 | The rotational spectrum and complete heavy atom structure of the chiral molecule verbenone. Journal of Molecular Spectroscopy, 2017, 342, 109-115. | 0.4 | 15 |
| 10924 | Radical Behavior of CO_2 versus its Deoxygenation Promoted by Vanadium Aryloxide Complexes: How the Geometry of Intermediate CO_2 Adducts Determines the Reactivity.. Chemistry - A European Journal, 2017, 23, 17269-17278. | 1.7 | 13 |
| 10925 | Infrared and density functional theory studies of isoprene-water complexes in noble gas matrices. Journal of Molecular Spectroscopy, 2017, 341, 27-34. | 0.4 | 3 |
| 10926 | Experimental and Computational Gas Phase Acidities of Conjugate Acids of Triazolylidene Carbenes: Rationalizing Subtle Electronic Effects. Journal of the American Chemical Society, 2017, 139, 14917-14930. | 6.6 | 33 |
| 10927 | Shedding Light on the Photoisomerization Pathway of Donor-Acceptor Stenhouse Adducts. Journal of the American Chemical Society, 2017, 139, 15596-15599. | 6.6 | 88 |
| 10928 | Noncovalent interactions underlying binary mixtures of amino acid based ionic liquids: insights from theory. Physical Chemistry Chemical Physics, 2017, 19, 29561-29582. | 1.3 | 1 |
| 10929 | Hidden complexities in the reaction of H_2O_2 and HNO revealed by ab initio quantum chemical investigations. Physical Chemistry Chemical Physics, 2017, 19, 29549-29560. | 1.3 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 10930 | 1,2-Fluorine Radical Rearrangements: Isomerization Events in Perfluorinated Radicals. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8675-8687. | 1.1 | 11 |
| 10931 | Doubling the power of DP4 for computational structure elucidation. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 8998-9007. | 1.5 | 53 |
| 10932 | Electron and nuclear spin polarization in Rb-Xe spin-exchange optical hyperpolarization. <i>Physical Review A</i> , 2017, 95, . | 1.0 | 6 |
| 10933 | Halide Abstraction Competes with Oxidative Addition in the Reactions of Aryl Halides with $[Ni(PMe_3)_4(Ph)(\eta^5-Cp^*)]$. <i>Chemistry - A European Journal</i> , 2017, 23, 16728-16733. | 1.7 | 46 |
| 10934 | Oxidation of Trialkylamines by $BrCCl_3$: Scope, Applications and Mechanistic Aspects. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 6966-6974. | 1.2 | 21 |
| 10935 | A Quantitative Analysis of Factors Influencing Ease of Formation and σ -Bonding Strength of Oxa- and Thia-N-Heterocyclic Carbenes. <i>Journal of Organic Chemistry</i> , 2017, 82, 12485-12491. | 1.7 | 15 |
| 10936 | Interrogating the Becke's ω density functional for non-locality information. <i>Journal of Chemical Physics</i> , 2017, 147, 154103. | 1.2 | 15 |
| 10937 | Reaction Coordinate Leading to H_2 Production in [FeFe]-Hydrogenase Identified by Nuclear Resonance Vibrational Spectroscopy and Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2017, 139, 16894-16902. | 6.6 | 78 |
| 10938 | Observation of promoted C=O bond weakening on the heterometallic nickel-silver: Photoelectron velocity-map imaging spectroscopy of $AgNi(CO)_2$. <i>Journal of Chemical Physics</i> , 2017, 146, 244316. | 1.2 | 10 |
| 10939 | Synthesis, Structures, and Characterization of Dimeric Neutral Dithiolato-bridged Tungsten Complexes. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 5434-5441. | 1.0 | 16 |
| 10940 | Band Gap in Magnetite above Verwey Temperature Induced by Symmetry Breaking. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25736-25742. | 1.5 | 73 |
| 10941 | Role of the Chalcogen (S, Se, Te) in the Oxidation Mechanism of the Glutathione Peroxidase Active Site. <i>ChemPhysChem</i> , 2017, 18, 2990-2998. | 1.0 | 46 |
| 10942 | Tautomerism and isomerism in some antitrichinellosis active benzimidazoles: Morphological study in polarized light, quantum chemical computations. <i>Journal of Molecular Structure</i> , 2017, 1150, 179-187. | 1.8 | 6 |
| 10943 | Tuning the Catalytic Alkyne Metathesis Activity of Molybdenum and Tungsten 2,4,6-Trimethylbenzylidene Complexes with Fluoroalkoxide Ligands $OC(CF_3)_3Me_3$ ($\eta^3 = \omega^3$). <i>Organometallics</i> , 2017, 36, 3398-3406. | 1.1 | 59 |
| 10944 | Why can a gold salt react as a base?. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 7841-7852. | 1.5 | 6 |
| 10945 | Molecular structure, nonlinear optical studies and spectroscopic analysis of chalcone derivative (2E)-3-[4-(methylsulfanyl) phenyl]-1-(3-bromophenyl) prop-2-en-1-one by DFT calculations. <i>Journal of Molecular Structure</i> , 2017, 1150, 166-178. | 1.8 | 33 |
| 10946 | Elucidating Substrate Promiscuity within the FabI Enzyme Family. <i>ACS Chemical Biology</i> , 2017, 12, 2465-2473. | 1.6 | 17 |
| 10947 | Intermetallic Cooperation in C-H Activation Involving Transient Titanium-Alkylidene Species: A Synthetic and Mechanistic Study. <i>Organometallics</i> , 2017, 36, 3076-3083. | 1.1 | 14 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10948 | Ab initio dynamics of unimolecular decomposition of β -propiolactone and β -propiolactam. <i>Chemical Physics Letters</i> , 2017, 686, 55-59. | 1.2 | 6 |
| 10949 | Importance of the alignment of polar π -conjugated molecules inside carbon nanotubes in determining second-order non-linear optical properties. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24819-24828. | 1.3 | 17 |
| 10950 | A low-cost approach to electronic excitation energies based on the driven similarity renormalization group. <i>Journal of Chemical Physics</i> , 2017, 147, 074107. | 1.2 | 12 |
| 10951 | Exploring Electrical Currents through Nanographenes: Visualization and Tuning of the through-Bond Transmission Paths. <i>ChemPhysChem</i> , 2017, 18, 3012-3022. | 1.0 | 23 |
| 10952 | Evaluating electronic structure methods for accurate calculation of ^{19}F chemical shifts in fluorinated amino acids. <i>Journal of Computational Chemistry</i> , 2017, 38, 2605-2617. | 1.5 | 12 |
| 10953 | Does low-energy collision-induced dissociation of lithiated and sodiated carbohydrates always occur at anomeric carbon of the reducing end?. <i>Rapid Communications in Mass Spectrometry</i> , 2017, 31, 1835-1844. | 0.7 | 24 |
| 10954 | Synthesis, characterization, computational and antimicrobial activities of a novel iridium thiourea complex. <i>New Journal of Chemistry</i> , 2017, 41, 10919-10928. | 1.4 | 9 |
| 10955 | Selective Recovery of Silver(I) Ions from E-Waste using Cubically Multithiolated Cage Mesoporous Monoliths. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 4823-4833. | 1.0 | 37 |
| 10956 | Synthesis, characterisation and in vitro cytotoxicity of mixed ligand Pt(II) oxadiazoline complexes with hexamethylenetetramine and 7-nitro-1,3,5-triazaadamantane. <i>Dalton Transactions</i> , 2017, 46, 12226-12238. | 1.6 | 6 |
| 10957 | Do fractionally incremented nuclear charges improve time-dependent density functional theory excitation energies as reliably as fractional orbital populations?. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1. | 0.5 | 1 |
| 10958 | Practical Density Functionals beyond the Overdelocalization-Underbinding Zero-Sum Game. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4314-4318. | 2.1 | 35 |
| 10959 | Reactions of (Cyclopentadienylidenehydrazono)triphenylphosphorane with Chlororuthenium(II) Complexes and Substituent Effect on the Thermodynamic Trend in the Migratory-Insertion Reactions of Chlororuthenium-Alkylidene Complexes. <i>Organometallics</i> , 2017, 36, 3266-3275. | 1.1 | 4 |
| 10960 | cis-Tetrachlorido-bis(indazole)osmium(IV) and its osmium(III) analogues: paving the way towards the cis-isomer of the ruthenium anticancer drugs KP1019 and/or NKP1339. <i>Dalton Transactions</i> , 2017, 46, 11925-11941. | 1.6 | 11 |
| 10961 | Photoactivatable CO-Releasing Properties of $\{\text{Ru}(\text{CO})_2\}$ -Core Pyridylbenzimidazole Complexes and Reactivity towards Lysozyme. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 4299-4310. | 1.0 | 21 |
| 10962 | Rhorix: An interface between quantum chemical topology and the 3D graphics program blender. <i>Journal of Computational Chemistry</i> , 2017, 38, 2538-2552. | 1.5 | 8 |
| 10963 | New heterometallic pivalates with Fe III and Zn II ions: Synthesis, structures, magnetic, thermal properties. <i>Polyhedron</i> , 2017, 137, 165-175. | 1.0 | 21 |
| 10964 | Metal-Assisted Ligand-Centered Electrocatalytic Hydrogen Evolution upon Reduction of a Bis(thiosemicarbazonato)Cu(II) Complex. <i>Inorganic Chemistry</i> , 2017, 56, 11254-11265. | 1.9 | 102 |
| 10965 | Rational Design of <i>in Vivo</i> Tau Tangle-Selective Near-Infrared Fluorophores: Expanding the BODIPY Universe. <i>Journal of the American Chemical Society</i> , 2017, 139, 13393-13403. | 6.6 | 117 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10966 | Porous graphene and graphenylene nanotubes: Electronic structure and strain effects. <i>Computational Materials Science</i> , 2017, 140, 344-355. | 1.4 | 10 |
| 10967 | A DFT study on the mechanism of Rh-catalyzed competitive 1,2- versus 1,3-acyloxy migration followed by [5+1] and [4+1] cycloadditions of 1,4-enynes with CO. <i>Journal of Organometallic Chemistry</i> , 2017, 851, 97-103. | 0.8 | 9 |
| 10968 | Charge Separation and Triplet Exciton Formation Pathways in Small-Molecule Solar Cells as Studied by Time-Resolved EPR Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2017, 121, 22707-22719. | 1.5 | 19 |
| 10969 | Generalized Optimized Effective Potential for Orbital Functionals and Self-Consistent Calculation of Random Phase Approximations. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4746-4751. | 2.1 | 18 |
| 10970 | 1'-Phthalazinylhydrazone of acetylferrocene: Structure, properties, and complexing ability. <i>Russian Journal of General Chemistry</i> , 2017, 87, 1759-1765. | 0.3 | 1 |
| 10971 | The trimerization of acetylenes involves a cascade of biradical and pericyclic processes. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 8326-8333. | 1.5 | 7 |
| 10972 | An acidic pH independent piperazine-TPPE AIEgen as a unique bioprobe for lysosome tracing. <i>Chemical Science</i> , 2017, 8, 7593-7603. | 3.7 | 112 |
| 10973 | Chromophores of chromophores: a bottom-up H ₂ ckel picture of the excited states of photoactive proteins. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29772-29779. | 1.3 | 24 |
| 10974 | The BioFragment Database (BFDdb): An open-data platform for computational chemistry analysis of noncovalent interactions. <i>Journal of Chemical Physics</i> , 2017, 147, 161727. | 1.2 | 82 |
| 10975 | Molecular Structure and Confining Environment of Sn Sites in Single-Site Chabazite Zeolites. <i>Chemistry of Materials</i> , 2017, 29, 8824-8837. | 3.2 | 44 |
| 10976 | Synthesis and Characterization of a Thiopyridazinylmethane-Based Scorpionate Ligand: Formation of Zinc Complexes and Rearrangement Reaction. <i>Organometallics</i> , 2017, 36, 3790-3798. | 1.1 | 8 |
| 10977 | Synthesis, structural characterization, thermal stability, vibrational spectra and density functional theoretical studies of 1,3-bis(carboxymethyl)imidazolium nitrate ionic liquid. <i>Journal of Molecular Liquids</i> , 2017, 246, 173-177. | 2.3 | 2 |
| 10978 | Benchmark of Dynamic Electron Correlation Models for Seniority-Zero Wave Functions and Their Application to Thermochemistry. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5966-5983. | 2.3 | 22 |
| 10979 | Dual Photochemical Reaction Pathway in Flavin-Based Photoreceptor LOV Domain: A Combined Quantum-Mechanics/Molecular-Mechanics Investigation. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9583-9596. | 1.2 | 14 |
| 10980 | Metastable exohedrally decorated Borospherene B40. <i>Scientific Reports</i> , 2017, 7, 7618. | 1.6 | 15 |
| 10981 | Bond dissociation energy controlled β -bond metathesis in alkaline-earth-metal hydride catalyzed dehydrocoupling of amines and boranes: a theoretical study. <i>Inorganic Chemistry Frontiers</i> , 2017, 4, 1813-1820. | 3.0 | 18 |
| 10982 | Spectroscopic investigations (FT-IR, UV, 1 H and 13 C NMR) and DFT/TD-DFT calculations of potential analgesic drug 2-[2-(dimethylamino)ethyl]-6-methoxy-4-(pyridin-2-yl)-1(2 H)-phthalazinone. <i>Journal of Molecular Structure</i> , 2017, 1150, 614-628. | 1.8 | 4 |
| 10983 | Triquinanes and Related Sesquiterpenes Revisited Computationally: Structure Corrections of Hirsutanols B and D, Hirsutenol E, Cucumin B, Antrodins C-E, Chondroterpenes A and H, Chondrosterins C and E, Dichrocephone A, and Pethybrene. <i>Journal of Organic Chemistry</i> , 2017, 82, 10795-10802. | 1.7 | 56 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 10984 | First-Principles Molecular Dynamics Analysis of Ligand-Free Suzuki–Miyaura Cross-Coupling in Water: Transmetalation and Reductive Elimination. <i>Journal of Physical Chemistry C</i> , 2017, 121, 19904-19914. | 1.5 | 9 |
| 10985 | A Rising Star: Truxene as a Promising Hole Transport Material in Perovskite Solar Cells. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21729-21739. | 1.5 | 32 |
| 10986 | Chiral Ramachandran Plots I: Glycine. <i>Biochemistry</i> , 2017, 56, 5635-5643. | 1.2 | 10 |
| 10987 | Catalytic mechanism of phenylacetone monooxygenases for non-native linear substrates. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26851-26861. | 1.3 | 11 |
| 10988 | Computational estimation of parity violation effects in a metal-organic framework containing DABCO. <i>Chemical Physics Letters</i> , 2017, 687, 110-115. | 1.2 | 6 |
| 10989 | Tetrasubstituted cyclopentadienones as suitable enantiopure ligands with axial chirality. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 8720-8728. | 1.5 | 3 |
| 10990 | Claisen rearrangements of benzyl vinyl ethers: theoretical investigation of mechanism, substituent effects, and regioselectivity. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 7887-7893. | 1.5 | 7 |
| 10991 | [Ni(bpy)(mal)(H ₂ O) ₃]·H ₂ O and [Ni(4,4'-dmbpy)(mal)(H ₂ O) ₃]·1.5H ₂ O: syntheses, crystal structures, magnetic properties, and computational study of stacking interactions. <i>Journal of Coordination Chemistry</i> , 2017, 70, 2999-3018. | 0.8 | 9 |
| 10992 | 1,2,3,4-Tetrahydroquinoline Arene Complexes as Intermediates in the Preparation of Molecular Phosphorescent Iridium(III) Complexes. <i>Chemistry - A European Journal</i> , 2017, 23, 15729-15737. | 1.7 | 22 |
| 10993 | Supramolecular complexes formed by dimethoxypillar[5]arenes and imidazolium salts: a joint experimental and computational investigation. <i>New Journal of Chemistry</i> , 2017, 41, 12490-12505. | 1.4 | 4 |
| 10994 | Tuning the Electronic Properties of Single-Atom Pt Catalysts by Functionalization of the Carbon Support Material. <i>Journal of Physical Chemistry C</i> , 2017, 121, 20802-20812. | 1.5 | 23 |
| 10995 | New Insights into the Catalytic Mechanism of Aldose Reductase: A QM/MM Study. <i>ACS Omega</i> , 2017, 2, 5737-5747. | 1.6 | 8 |
| 10996 | Lissodendoric Acids A and B, Manzamine-Related Alkaloids from the Far Eastern Sponge <i>Lissodendoryx florida</i> . <i>Organic Letters</i> , 2017, 19, 5320-5323. | 2.4 | 15 |
| 10997 | Computational design of bio-inspired carnosine-based HOBr antioxidants. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 905-913. | 1.3 | 8 |
| 10998 | Methane C–H Activation via 3d Metal Methoxide Complexes with Potentially Redox-Noninnocent Pincer Ligands: A Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2017, 56, 12282-12290. | 1.9 | 17 |
| 10999 | Energetics and mechanism of anion permeation across formate-nitrite transporters. <i>Scientific Reports</i> , 2017, 7, 12027. | 1.6 | 32 |
| 11000 | Ab Initio Computation of Energy Deposition During Electron Ionization of Molecules. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7751-7760. | 1.1 | 10 |
| 11001 | A study of size-dependent properties of MoS ₂ monolayer nanoflakes using density-functional theory. <i>Scientific Reports</i> , 2017, 7, 9775. | 1.6 | 30 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11002 | Conformational Preference and Spectroscopical Characteristics of the Active Pharmaceutical Ingredient Levetiracetam. <i>Journal of Pharmaceutical Sciences</i> , 2017, 106, 3564-3573. | 1.6 | 2 |
| 11003 | Energetics of Baird aromaticity supported by inversion of photoexcited chiral [4n]annulene derivatives. <i>Nature Communications</i> , 2017, 8, 346. | 5.8 | 86 |
| 11004 | Predicting the Ionic Product of Water. <i>Scientific Reports</i> , 2017, 7, 10244. | 1.6 | 40 |
| 11005 | Optical Properties of Small Gold Clusters Au ₈ L ₈ 2 ⁺ (L = PH ₃ , PPh ₃): Magnetic Circular Dichroism Spectra. <i>Journal of Physical Chemistry C</i> , 2017, 121, 19478-19489. | 1.5 | 15 |
| 11006 | Paramagnetism in Metallocarboranes: The Polyhedral Chromadiborane Systems. <i>Inorganic Chemistry</i> , 2017, 56, 11059-11065. | 1.9 | 2 |
| 11007 | Effects of different proton donor and acceptor groups on excited-state intramolecular proton transfers of amino-type and hydroxy-type hydrogen-bonding molecules: theoretical insights. <i>New Journal of Chemistry</i> , 2017, 41, 8761-8771. | 1.4 | 46 |
| 11008 | The first water coordination sphere of lanthanide(III) motexafins (Ln-Motex2+, Ln = La, Gd, Lu) and its effects on structures, reduction potentials and UV-vis absorption spectra. Theoretical studies. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 20160-20171. | 1.3 | 9 |
| 11009 | A Computational Study of the Intermolecular [2+2+2] Cycloaddition of Acetylene and C ₆₀ Catalyzed by Wilkinson's Catalyst. <i>Chemistry - A European Journal</i> , 2017, 23, 15067-15072. | 1.7 | 11 |
| 11010 | Aryl-Substituted Ruthenium(II) Complexes: A Strategy for Enhanced Photocleavage and Efficient DNA Binding. <i>Inorganic Chemistry</i> , 2017, 56, 9084-9096. | 1.9 | 39 |
| 11011 | Multiscale Simulations on Charge Transport in Covalent Organic Frameworks Including Dynamics of Transfer Integrals from the FMO-DFTB/LCMO Approach. <i>Journal of Physical Chemistry C</i> , 2017, 121, 17712-17726. | 1.5 | 16 |
| 11012 | Catalytic and Enantioselective Diels-Alder Reactions of (E)-4-Oxopent-2-enoates. <i>Organic Letters</i> , 2017, 19, 3986-3989. | 2.4 | 17 |
| 11013 | Theoretical tuning of the singlet-triplet energy gap to achieve efficient long-wavelength thermally activated delayed fluorescence emitters: the impact of substituents. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21639-21647. | 1.3 | 14 |
| 11014 | Photochromic coenzyme Q derivatives: switching redox potentials with light. <i>Chemical Science</i> , 2017, 8, 6474-6483. | 3.7 | 27 |
| 11015 | Excited state absorption spectra of dissolved and aggregated distyrylbenzene: A TD-DFT state and vibronic analysis. <i>Journal of Chemical Physics</i> , 2017, 147, 034903. | 1.2 | 17 |
| 11016 | Mechanistic insights into the biomimetic catalytic hydroxylation of arenes by a molecular Fe(NHC) complex. <i>Journal of Catalysis</i> , 2017, 352, 599-605. | 3.1 | 13 |
| 11017 | Theoretical study on photochemistry of Irgacure 907. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 347, 78-85. | 2.0 | 11 |
| 11018 | Assignment of solid-state ¹³ C and ¹ H NMR spectra of paramagnetic Ni(II) acetylacetonate complexes aided by first-principles computations. <i>Solid State Nuclear Magnetic Resonance</i> , 2017, 87, 29-37. | 1.5 | 17 |
| 11019 | Model for the Enantioselectivity of Asymmetric Intramolecular Alkylations by Bis-Quaternized Cinchona Alkaloid-Derived Catalysts. <i>Journal of Organic Chemistry</i> , 2017, 82, 8645-8650. | 1.7 | 29 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11020 | Simulated Mechanism for Palladium-Catalyzed, Directed \hat{I}^3 -Arylation of Piperidine. ACS Catalysis, 2017, 7, 5466-5477. | 5.5 | 33 |
| 11021 | Collision-induced dissociation of sodiated glucose and identification of anomeric configuration. Physical Chemistry Chemical Physics, 2017, 19, 15454-15462. | 1.3 | 46 |
| 11022 | Enhanced Luminescence of Asymmetrical Seven-coordinate Eu^{III} Complexes Including LMCT Perturbation. European Journal of Inorganic Chemistry, 2017, 2017, 3843-3848. | 1.0 | 53 |
| 11023 | Regioselectivity in the hetero-Diels-Alder reactions of styrenes with 2-aza-1,3-butadiene: a DFT study. Journal of Chemical Sciences, 2017, 129, 1319-1325. | 0.7 | 1 |
| 11024 | Computational Approaches to the Study of Melanogenesis. , 2017, , 227-238. | | 0 |
| 11025 | Trifluoromethylation of a Well-Defined Square-Planar Aryl- Ni^{II} Complex involving $\text{Ni}^{\text{III}}/\text{CF}_3$ and $\text{Ni}^{\text{IV}}/\text{CF}_3$ Intermediate Species. Chemistry - A European Journal, 2017, 23, 11662-11668. | 1.7 | 23 |
| 11026 | Extension of the D3 dispersion coefficient model. Journal of Chemical Physics, 2017, 147, 034112. | 1.2 | 617 |
| 11027 | Benchmarking density functional tight binding models for barrier heights and reaction energetics of organic molecules. Journal of Computational Chemistry, 2017, 38, 2171-2185. | 1.5 | 39 |
| 11028 | Prediction of the lowest charge-transfer excited-state energy at the donor-acceptor interface in a condensed phase using ground-state DFT calculations with generalized Kohn-Sham functionals. Journal of Molecular Modeling, 2017, 23, 235. | 0.8 | 11 |
| 11029 | Growth of polycyclic aromatic hydrocarbons (PAHs) by methyl radicals: Pyrene formation from phenanthrene. Combustion and Flame, 2017, 185, 129-141. | 2.8 | 35 |
| 11030 | Spin-Dependent Exciton Funneling to a Dendritic Fluorophore Mediated by a Thermally Activated Delayed Fluorescence Material as an Exciton-Harvesting Host. Chemistry of Materials, 2017, 29, 7014-7022. | 3.2 | 53 |
| 11031 | Electronic and Optical Properties of Methylated Adamantanes. Journal of the American Chemical Society, 2017, 139, 11132-11137. | 6.6 | 13 |
| 11032 | Asymmetric Hydrogen Bonding Catalysis for the Synthesis of Dihydroquinazoline-Containing Antiviral, Letemovir. Journal of the American Chemical Society, 2017, 139, 10637-10640. | 6.6 | 28 |
| 11033 | Nonconventional screening of the Coulomb interaction in $\langle \text{O} \rangle$ clusters: An <i>ab initio</i> study. Physical Review B, 2017, 95, . | 1.1 | 14 |
| 11034 | A theoretical study on [2+2] cycloaddition reactions under visible light irradiation induced by energy transfer. Computational and Theoretical Chemistry, 2017, 1117, 47-54. | 1.1 | 2 |
| 11035 | Gallium Complexation, Stability, and Bioconjugation of 1,4,7-Triazacyclononane Derived Chelators with Azaheterocyclic Arms. Inorganic Chemistry, 2017, 56, 9097-9110. | 1.9 | 25 |
| 11036 | Density Functional Theory Assessment of the Environment Polarity Effect on Polyaniline-Water Coupling. Journal of Physical Chemistry A, 2017, 121, 6327-6335. | 1.1 | 1 |
| 11037 | Structure and reactivity of $[\text{Ru}^{\text{II}}(\text{terpy})(\text{N}^{\wedge}\text{N})\text{Cl}]\text{Cl}$ complexes: consequences for biological applications. Dalton Transactions, 2017, 46, 10264-10280. | 1.6 | 24 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11038 | Revised M06-L functional for improved accuracy on chemical reaction barrier heights, noncovalent interactions, and solid-state physics. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 8487-8492. | 3.3 | 167 |
| 11039 | Comparative first-principles studies of prototypical ferroelectric materials by LDA, GGA, and SCAN meta-GGA. Physical Review B, 2017, 96, . | 1.1 | 156 |
| 11040 | Enantioresolution and stereochemical characterization of two chiral sulfoxides endowed with COX α 2 inhibitory activity. Chirality, 2017, 29, 536-540. | 1.3 | 11 |
| 11041 | Pyranose ring conformations in mono- and oligosaccharides: a combined MD and DFT approach. Physical Chemistry Chemical Physics, 2017, 19, 20760-20772. | 1.3 | 18 |
| 11042 | Spectroscopic Observation of the Triplet Diradical State of a Cyclobutadiene. Angewandte Chemie, 2017, 129, 10317-10321. | 1.6 | 13 |
| 11043 | Engineering electronic structure of a fullerene C 20 bowl with germanium impurities. Chinese Journal of Physics, 2017, 55, 2134-2143. | 2.0 | 15 |
| 11044 | Structure, thermal stability, antioxidant activity and DFT studies of trisphenols and related phenols. Inorganica Chimica Acta, 2017, 468, 159-170. | 1.2 | 19 |
| 11045 | Pronounced conformational flexibility of physiological (l-histidinato)(l-threoninato)copper(II) in aqueous solution disclosed by a quantum chemical study. Polyhedron, 2017, 135, 121-133. | 1.0 | 4 |
| 11046 | Assessment of Tuned Range Separated Exchange Functionals for Spectroscopies and Properties of Uranium Complexes. Journal of Chemical Theory and Computation, 2017, 13, 3614-3625. | 2.3 | 17 |
| 11047 | Regioselective Diversification of 2,1-Borazaronaphthalenes: Unlocking Isosteric Space via C-H Activation. Journal of Organic Chemistry, 2017, 82, 8072-8084. | 1.7 | 24 |
| 11048 | 8OCB and 8CB Liquid Crystals Confined in Nanoporous Alumina: Effect of Confinement on the Structure and Dynamics. Journal of Physical Chemistry B, 2017, 121, 7382-7394. | 1.2 | 25 |
| 11049 | Competing Annulene and Radialene Structures in a Single Anti-Aromatic Molecule Studied by High-Resolution Atomic Force Microscopy. ACS Nano, 2017, 11, 8122-8130. | 7.3 | 64 |
| 11050 | A non-empirical calculation of 2p core-electron excitation in compounds with 3d transition metal ions using ligand-field and density functional theory (LFDFT). Physical Chemistry Chemical Physics, 2017, 19, 20919-20929. | 1.3 | 15 |
| 11051 | Pyrene Molecular Orbital Shuffle—Controlling Excited State and Redox Properties by Changing the Nature of the Frontier Orbitals. Chemistry - A European Journal, 2017, 23, 13164-13180. | 1.7 | 90 |
| 11052 | On Atoms' Molecules Energies from Kohn-Sham Calculations. ChemPhysChem, 2017, 18, 2675-2687. | 1.0 | 29 |
| 11053 | ETS-NOCV Decomposition of the Reaction Force: The HCN/CNH Isomerization Reaction Assisted by Water. Journal of Computational Chemistry, 2017, 38, 2076-2087. | 1.5 | 19 |
| 11054 | An efficient strategy for designing ambipolar organic semiconductor material: Introducing dehydrogenated phosphorus atoms into pentacene core. Chemical Physics Letters, 2017, 684, 402-408. | 1.2 | 4 |
| 11055 | Novel derivatives of regioisomerically pure 1,7-disubstituted perylene diimide dyes bearing phenoxy and pyrrolidinyl substituents: Synthesis, photophysical, thermal, and structural properties. Journal of Luminescence, 2017, 192, 414-423. | 1.5 | 13 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11056 | A comprehensive test of computational approaches for evaluation of cyclodextrin complexes. Self-inclusion in monosubstituted β -cyclodextrins – a case study. <i>Tetrahedron</i> , 2017, 73, 5302-5306. | 1.0 | 3 |
| 11057 | Thermal isomerization of azobenzenes: on the performance of Eyring transition state theory. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 314002. | 0.7 | 19 |
| 11058 | Insights into the Hydrogen-Atom Transfer of the Blue AroxyI. <i>ChemPhysChem</i> , 2017, 18, 2932-2938. | 1.0 | 0 |
| 11059 | Temperature-Dependent Dynamics of Push-Pull Rotor Systems Based on Acridinylidene Cyanoacetic Esters. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 5141-5146. | 1.2 | 6 |
| 11060 | Tautomerism-Induced Cis-Trans Isomerization of Pyridylethenyl N-Confused Porphyrin. <i>Journal of Organic Chemistry</i> , 2017, 82, 8686-8696. | 1.7 | 20 |
| 11061 | Oxazine Ring-Related Vibrational Modes of Benzoxazine Monomers Using Fully Aromatically Substituted, Deuterated, ^{15}N Isotope Exchanged, and Oxazine-Ring-Substituted Compounds and Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6269-6282. | 1.1 | 198 |
| 11062 | Using non-empirically tuned range-separated functionals with simulated emission bands to model fluorescence lifetimes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21046-21057. | 1.3 | 12 |
| 11063 | Bismuth nitrate-promoted disproportionative condensation of indoles with cyclohexanone: a new-type azafulvenium reactivity of indole. <i>New Journal of Chemistry</i> , 2017, 41, 9674-9687. | 1.4 | 7 |
| 11064 | The phosphorescence properties of a series of diarylethene-containing platinum complexes: the effect of ligand photoisomerization. <i>Organic Chemistry Frontiers</i> , 2017, 4, 2191-2201. | 2.3 | 11 |
| 11065 | Intramolecular alkyne-dithiolium cycloaddition: a joint experimental and DFT mechanistic study. <i>RSC Advances</i> , 2017, 7, 36623-36631. | 1.7 | 5 |
| 11066 | Density Functional Calculations for Prediction of ^{57}Fe Mössbauer Isomer Shifts and Quadrupole Splittings in β -Diketiminato Complexes. <i>ACS Omega</i> , 2017, 2, 2594-2606. | 1.6 | 37 |
| 11067 | Nucleophilic Aromatic Addition in Ionizing Environments: Observation and Analysis of New C-N Valence Bonds in Complexes between Naphthalene Radical Cation and Pyridine. <i>Journal of the American Chemical Society</i> , 2017, 139, 11923-11932. | 6.6 | 11 |
| 11068 | TFSI and TDI Anions: Probes for Solvate Ionic Liquid and Disproportionation-Based Lithium Battery Electrolytes. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3678-3682. | 2.1 | 21 |
| 11069 | Targeted radionuclide therapy with astatine-211: Oxidative dehalogenation of astatobenzoate conjugates. <i>Scientific Reports</i> , 2017, 7, 2579. | 1.6 | 45 |
| 11070 | Prediction of hypervalent molecules: investigation on M_nC (M = Li, Na, K, Rb and Cs; n =) <small>Tj ETQq0 0 0,rgBT /Overlock 10 TF</small> | 1.8 | 9 |
| 11071 | Low-spin $[\text{M}^{\text{II}}(\text{L})_2]$ and $[\text{M}^{\text{III}}(\text{L})_2]^{+}$ (M = Fe) <small>Tj ETQq1 1 0.784314 rgBT</small> and redox potential correlations. <i>Dalton Transactions</i> , 2017, 46, 11291-11305. | 1.6 | 12 |
| 11072 | A Direct Link from the Gas to the Condensed Phase: A Rotational Spectroscopic Study of 2,2,2-Trifluoroethanol Trimers. <i>Angewandte Chemie</i> , 2017, 129, 6386-6390. | 1.6 | 31 |
| 11073 | Porphyrins Conjugated with Peripheral Thiolato Gold(I) Complexes for Enhanced Photodynamic Therapy. <i>Chemistry - A European Journal</i> , 2017, 23, 14017-14026. | 1.7 | 37 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11074 | Bias-Free Chemically Diverse Test Sets from Machine Learning. <i>ACS Combinatorial Science</i> , 2017, 19, 544-554. | 3.8 | 10 |
| 11075 | Glutamate Water Gates in the Ion Binding Pocket of Na ⁺ Bound Na ⁺ , K ⁺ -ATPase. <i>Scientific Reports</i> , 2017, 7, 39829. | 1.6 | 8 |
| 11076 | Assessment of two hybrid van der Waals density functionals for covalent and non-covalent binding of molecules. <i>Journal of Chemical Physics</i> , 2017, 146, 234106. | 1.2 | 33 |
| 11077 | Efficient local-orbitals based method for ultrafast dynamics. <i>Journal of Chemical Physics</i> , 2017, 147, 044111. | 1.2 | 4 |
| 11078 | Synthese, Struktur und Bindungsanalyse eines homoleptischen Berylliumazids. <i>Angewandte Chemie</i> , 2017, 129, 8680-8685. | 1.6 | 7 |
| 11079 | Optimizing the Accuracy and Computational Cost in Theoretical Squaramide Catalysis: The Henry Reaction. <i>Chemistry - A European Journal</i> , 2017, 23, 15336-15347. | 1.7 | 18 |
| 11080 | Computational modeling of strained alkenes: Choosing the right computational model. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25439. | 1.0 | 5 |
| 11081 | Rhodium-Catalyzed [2+2+2] Cycloaddition Reactions of Linear Allene-Ynes to afford Fused Tricyclic Scaffolds: Insights into the Mechanism. <i>Chemistry - A European Journal</i> , 2017, 23, 14889-14899. | 1.7 | 22 |
| 11082 | Heme isomers substantially affect heme's electronic structure and function. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 22355-22362. | 1.3 | 14 |
| 11083 | Cyclopropyl Group: An Excited-State Aromaticity Indicator?. <i>Chemistry - A European Journal</i> , 2017, 23, 13684-13695. | 1.7 | 10 |
| 11084 | Gold(I)-Alkynyl Complexes with an N-Donor Heterocyclic Ligand: Synthesis and Photophysical Properties. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 4180-4186. | 1.0 | 11 |
| 11085 | The bonding picture in hypervalent XF ₃ (X=Cl, Br, I, At) fluorides revisited with quantum chemical topology. <i>Journal of Computational Chemistry</i> , 2017, 38, 2753-2762. | 1.5 | 11 |
| 11086 | Polymethylene-b-poly (acrylic acid) diblock copolymers: Aggregation and crystallization in the presence of CaCl ₂ . <i>European Polymer Journal</i> , 2017, 95, 174-185. | 2.6 | 14 |
| 11087 | Linear-Response Time-Dependent Embedded Mean-Field Theory. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4216-4227. | 2.3 | 20 |
| 11088 | Self-interaction effects on charge-transfer collisions. <i>Physical Review A</i> , 2017, 95, . | 1.0 | 20 |
| 11089 | Accurate potential energy surfaces for hydrogen abstraction reactions: A benchmark study on the XYG3 doubly hybrid density functional. <i>Journal of Computational Chemistry</i> , 2017, 38, 2326-2334. | 1.5 | 4 |
| 11090 | Computational study of fluoroquinolone binding to Mg(H ₂ O) ₆ ²⁺ and its applicability to future drug design. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25428. | 1.0 | 5 |
| 11091 | An Aerobic Synthetic Approach toward Bis-Alkynyl Cobalt(III) Compounds. <i>Inorganic Chemistry</i> , 2017, 56, 10021-10031. | 1.9 | 14 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11092 | Remarkable nonlinear optical response of excess electron compounds: theoretically designed alkali-doped aziridine $(C_2NH_5)_n$. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 23951-23959. | 1.3 | 25 |
| 11093 | A QM/MM study to investigate selectivity of nanoporous graphene membrane for arsenate and chromate removal from water. <i>Chemical Physics Letters</i> , 2017, 685, 371-376. | 1.2 | 7 |
| 11094 | Molybdenum Trihydride Complexes: Computational Model of Oxidatively Induced Reductive Elimination of Dihydrogen. <i>Inorganic Chemistry</i> , 2017, 56, 9653-9659. | 1.9 | 2 |
| 11095 | Germanium and Tin Monoxides Trapped by Oxophilic Germylene and Stannylene Ligands. <i>Inorganic Chemistry</i> , 2017, 56, 10220-10225. | 1.9 | 7 |
| 11096 | Phosphinous Acid-Assisted Hydration of Nitriles: Understanding the Controversial Reactivity of Osmium and Ruthenium Catalysts. <i>Chemistry - A European Journal</i> , 2017, 23, 15210-15221. | 1.7 | 44 |
| 11097 | Nucleophilicity and electrophilicity of the $C(sp^3)H$ bond: methane and ethane binary complexes with iodine. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24555-24565. | 1.3 | 3 |
| 11098 | Chemoselective oxidation of unsaturated organosulfur, selenium and phosphorus compounds by molybdenum oxodiperoxo complexes: A computational investigation. <i>Inorganica Chimica Acta</i> , 2017, 467, 351-357. | 1.2 | 4 |
| 11099 | Why do zeolites induce an unprecedented electronic state on exchanged metal ions?. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 25105-25114. | 1.3 | 11 |
| 11100 | Calix[4]arene-fused phospholes. <i>Dalton Transactions</i> , 2017, 46, 9833-9845. | 1.6 | 19 |
| 11101 | Assessment of long-range-corrected exchange-correlation kernels for solids: Accurate exciton binding energies via an empirically scaled bootstrap kernel. <i>Physical Review B</i> , 2017, 95, . | 1.1 | 31 |
| 11102 | Observed adducts on positive mode direct analysis in real time mass spectrometry – Proton/ammonium adduct selectivities of 600-sample in-house chemical library. <i>European Journal of Mass Spectrometry</i> , 2017, 23, 4-10. | 0.5 | 9 |
| 11103 | Synthesis, molecular structure, vibrational spectroscopy, optical investigation and DFT study of a novel hybrid material: 3,3'-diammoniumdiphenylsulfone hexachloridostannate monohydrate. <i>Journal of Molecular Structure</i> , 2017, 1149, 818-827. | 1.8 | 23 |
| 11104 | Regioselective Hydrogenolysis of Donor-Acceptor Cyclopropanes with Zn-AcOH Reductive System. <i>Journal of Organic Chemistry</i> , 2017, 82, 9537-9549. | 1.7 | 16 |
| 11105 | Accurate Valence Ionization Energies from Kohn-Sham Eigenvalues with the Help of Potential Adjustors. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4726-4740. | 2.3 | 11 |
| 11106 | The Many Facets of Chalcogen Bonding: Described by Vibrational Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6845-6862. | 1.1 | 95 |
| 11107 | Importance of the ligand basis set in ab initio thermochemical calculations of transition metal species. <i>Chemical Physics Letters</i> , 2017, 685, 496-503. | 1.2 | 2 |
| 11108 | The structural landscape in 14-vertex clusters of silicon, $M@Si_{14}$: when two bonding paradigms collide. <i>Dalton Transactions</i> , 2017, 46, 11636-11644. | 1.6 | 19 |
| 11109 | Why are GCAs so accurate for reaction kinetics on surfaces? Systematic comparison of hybrid vs. nonhybrid DFT for representative reactions. <i>Journal of Chemical Physics</i> , 2017, 146, 234103. | 1.2 | 11 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11110 | Performance of a nonempirical exchange functional from density matrix expansion: comparative study with different correlations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21707-21713. | 1.3 | 20 |
| 11111 | Novel non-spherical deltahedra in tritungstaboranes related to the experimentally known $Cp^*W_3(H)B_8H_8$. <i>New Journal of Chemistry</i> , 2017, 41, 10640-10651. | 1.4 | 4 |
| 11112 | Valence electronic structure of cobalt phthalocyanine from an optimally tuned range-separated hybrid functional. <i>Journal of Chemical Physics</i> , 2017, 147, 044301. | 1.2 | 48 |
| 11113 | Theoretical design of new class of optical materials based on small noble metal nanocluster-biomolecule hybrids and its potential for medical applications. <i>Advances in Physics: X</i> , 2017, 2, 695-716. | 1.5 | 6 |
| 11114 | Structure and dynamics of CaO films: A computational study of an effect of external static electric field. <i>Physical Review B</i> , 2017, 95, . | 1.1 | 2 |
| 11115 | Wannier Koopman method calculations of the band gaps of alkali halides. <i>Applied Physics Letters</i> , 2017, 111, . | 1.5 | 10 |
| 11116 | Crystal structure of (2Z)-(3,3-dimethyl-3,4-dihydroisoquinolin-1(2H)-ylidene)nitrosoacetonitrile. <i>Crystallography Reports</i> , 2017, 62, 566-571. | 0.1 | 0 |
| 11117 | Adsorption and coadsorption mechanisms of Cr(VI) and organic contaminants on H ₃ PO ₄ treated biochar. <i>Chemosphere</i> , 2017, 186, 422-429. | 4.2 | 133 |
| 11118 | Best methods for calculating interaction energies in 2-butene and butane systems. <i>Computational and Theoretical Chemistry</i> , 2017, 1117, 150-161. | 1.1 | 3 |
| 11119 | Sol-Gel auto-combustion synthesis and physicochemical properties of BaAl ₂ O ₄ nanoparticles; electrochemical hydrogen storage performance and density functional theory. <i>Renewable Energy</i> , 2017, 114, 1419-1426. | 4.3 | 44 |
| 11120 | Assessing Excited State Energy Gaps with Time-Dependent Density Functional Theory on Ru(II) Complexes. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4123-4145. | 2.3 | 39 |
| 11121 | A five-coordinate manganese(III) complex of a salen type ligand with a positive axial anisotropy parameter D. <i>Dalton Transactions</i> , 2017, 46, 11817-11829. | 1.6 | 20 |
| 11122 | Characterization of Local Aromaticity in Polycyclic Conjugated Hydrocarbons Based on Anisotropy of π -Electron Density. <i>ChemistrySelect</i> , 2017, 2, 11526-11536. | 0.7 | 3 |
| 11123 | To Be Bridgehead or Not to Be? This is a Question of Metallabicycles on the Interplay between Aromaticity and Ring Strain. <i>Organometallics</i> , 2017, 36, 4896-4900. | 1.1 | 9 |
| 11124 | New insights into the mechanism of nickel superoxide degradation from studies of model peptides. <i>Scientific Reports</i> , 2017, 7, 17194. | 1.6 | 16 |
| 11125 | A combined electronic structure and molecular dynamics approach to computing the OH vibrational feature of strongly hydrogen-bonded carboxylic acids. <i>Journal of Chemical Physics</i> , 2017, 147, 224304. | 1.2 | 12 |
| 11126 | Machine learning unifies the modeling of materials and molecules. <i>Science Advances</i> , 2017, 3, e1701816. | 4.7 | 488 |
| 11127 | Assessing the performance of self-consistent hybrid functional for band gap calculation in oxide semiconductors. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 454004. | 0.7 | 33 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11128 | How Interatomic Steps in the Exact Kohn-Sham Potential Relate to Derivative Discontinuities of the Energy. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5974-5980. | 2.1 | 43 |
| 11129 | Metal-Center-Driven Supramolecular Chirogenesis in <i><i>Tweezer</i></i> Amino Alcohol Complexes: Structural, Spectroscopic, and Theoretical Investigations. <i>Inorganic Chemistry</i> , 2017, 56, 15203-15215. | 1.9 | 17 |
| 11130 | Extending density functional embedding theory for covalently bonded systems. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E10861-E10870. | 3.3 | 21 |
| 11131 | Prediction of metabolites of epoxidation reaction in MetaTox. SAR and QSAR in Environmental Research, 2017, 28, 833-842. | 1.0 | 12 |
| 11132 | Donor-Acceptor Strategies for Stabilizing Planar Diplumbenes. <i>Organometallics</i> , 2017, 36, 4825-4833. | 1.1 | 3 |
| 11133 | Crystal phase transition of urea: what governs the reaction kinetics in molecular crystal phase transitions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32125-32131. | 1.3 | 10 |
| 11134 | Efficient ¹ H NMR chiral discrimination of sulfoxides caused by the dynamic nature of (R,R)-3,3'-biBINOL. <i>Tetrahedron: Asymmetry</i> , 2017, 28, 1587-1590. | 1.8 | 1 |
| 11135 | Bioinspired graphene membrane with temperature tunable channels for water gating and molecular separation. <i>Nature Communications</i> , 2017, 8, 2011. | 5.8 | 175 |
| 11136 | Characterization of Silicon Nanocrystal Surfaces by Multidimensional Solid-State NMR Spectroscopy. <i>Chemistry of Materials</i> , 2017, 29, 10339-10351. | 3.2 | 37 |
| 11137 | Electronic structure and dynamics of torsion-locked photoactive yellow protein chromophores. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31572-31580. | 1.3 | 12 |
| 11138 | Nitro derivatives of pyrrolo[3,2-d]pyrimidine-2,4-diones: Synthesis of amines and new polynuclear heterocycles based thereon. <i>Russian Journal of Organic Chemistry</i> , 2017, 53, 1564-1572. | 0.3 | 3 |
| 11139 | Can Carbamates Undergo Radical Oxidation in the Soil Environment? A Case Study on Carbaryl and Carbofuran. <i>Environmental Science & Technology</i> , 2017, 51, 14124-14134. | 4.6 | 15 |
| 11140 | Cryptophanes for Methane and Xenon Encapsulation: A Comparative Density Functional Theory Study of Binding Properties and NMR Chemical Shifts. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9669-9677. | 1.1 | 8 |
| 11141 | Reversible switching of the spin state in a manganese phthalocyanine molecule by atomic nitrogen. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32655-32662. | 1.3 | 7 |
| 11142 | A note on the accuracy of KS-DFT densities. <i>Journal of Chemical Physics</i> , 2017, 147, 204103. | 1.2 | 23 |
| 11143 | Photoelectron spectra and electronic structure of nitrogen-containing chelate boron complexes. <i>Journal of Structural Chemistry</i> , 2017, 58, 1069-1078. | 0.3 | 4 |
| 11144 | Ground-State Gas-Phase Structures of Inorganic Molecules Predicted by Density Functional Theory Methods. <i>ACS Omega</i> , 2017, 2, 8373-8387. | 1.6 | 14 |
| 11145 | Theoretical calculation pKa values of phthalhydrazide derivatives in its aqueous solutions. <i>Russian Journal of Physical Chemistry B</i> , 2017, 11, 722-728. | 0.2 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11146 | Fluorescent vinyl and styryl coumarins: A comprehensive DFT study of structural, electronic and NLO properties. <i>Journal of Chemical Sciences</i> , 2017, 129, 1829-1841. | 0.7 | 24 |
| 11147 | Synthesis and Reactivity of a Low-Coordinate Iron(II) Hydride Complex: Applications in Catalytic Hydrodefluorination. <i>Inorganic Chemistry</i> , 2017, 56, 14513-14523. | 1.9 | 17 |
| 11148 | Origins of Enantioselectivity in Asymmetric Radical Additions to Octahedral Chiral-at-Rhodium Enolates: A Computational Study. <i>Journal of the American Chemical Society</i> , 2017, 139, 17902-17907. | 6.6 | 58 |
| 11149 | On the calculation of multiplet energies of three-open-shell $4f^{13}5f^n6d^1$ electron configuration by LFDFT: modeling the optical spectra of 4f core-electron excitation in actinide compounds. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32481-32491. | 1.3 | 8 |
| 11150 | Electronic Structure of Anilinopyridinate-Supported Ru^{2+5+} Paddlewheel Compounds. <i>Inorganic Chemistry</i> , 2017, 56, 14662-14670. | 1.9 | 13 |
| 11151 | Benzo[<i>b</i>]thiophene Fusion Enhances Local Borepin Aromaticity in Polycyclic Heteroaromatic Compounds. <i>Journal of Organic Chemistry</i> , 2017, 82, 13440-13448. | 1.7 | 37 |
| 11152 | Covalent Bonding in the Hydrogen Molecule. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9330-9345. | 1.1 | 15 |
| 11153 | The benchmark of ^{31}P NMR parameters in phosphate: a case study on structurally constrained and flexible phosphate. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31830-31841. | 1.3 | 17 |
| 11154 | Quantum Chemical Simulation of the Interaction of Functional Groups in Polyurethanes with 3d-Metal Ions During Their Extraction from Aqueous Solutions. <i>Journal of Applied Spectroscopy</i> , 2017, 84, 816-823. | 0.3 | 1 |
| 11155 | Computational and Experimental Study of Thermodynamics of the Reaction of Titania and Water at High Temperatures. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9508-9517. | 1.1 | 19 |
| 11156 | Which is the Stronger Nucleophile, Platinum or Nitrogen in Rollover Cycloplatinated(II) Complexes?. <i>Inorganic Chemistry</i> , 2017, 56, 14706-14713. | 1.9 | 11 |
| 11157 | A Simple Method of Predicting Spin State in Solution. <i>Journal of the American Chemical Society</i> , 2017, 139, 18392-18396. | 6.6 | 68 |
| 11158 | Ruthenium Carbon-Rich Group as a Redox-Switchable Metal Coupling Unit in Linear Trinuclear Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 14540-14555. | 1.9 | 9 |
| 11159 | Ligand Substituent Effects in Manganese Pyridinophane Complexes: Implications for Oxygen-Evolving Catalysis. <i>Inorganic Chemistry</i> , 2017, 56, 14315-14325. | 1.9 | 22 |
| 11160 | The effect of structural modifications on the thermal stability, melting points and ion interactions for a series of tetraaryl-phosphonium-based mesothermal ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31560-31571. | 1.3 | 19 |
| 11161 | Coordination and Insertion: Competitive Channels for Borylene Reactions. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8982-8994. | 1.1 | 4 |
| 11162 | Computational study of selectivity in the $[Pt^{II}Cl_4]^{2-}$ -catalysed arylation of arenes by diaryliodonium reagents: arene activation at Pt^{IV} centres. <i>Dalton Transactions</i> , 2017, 46, 15480-15486. | 1.6 | 6 |
| 11163 | Trends in Strong Chemical Bonding in C_2 , CN, CN^{\ominus} , CO, N_2 , NO, NO^+ , and O_2 . <i>Journal of Physical Chemistry A</i> , 2017, 121, 9092-9098. | 1.1 | 19 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11164 | Fast optical work-function tuning at an organic/metal interface. <i>Applied Physics Letters</i> , 2017, 111, 081601. | 1.5 | 5 |
| 11165 | Simultaneous Introduction of Two Nitroxides in the Reaction: A New Approach to the Synthesis of Heterospin Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 14567-14576. | 1.9 | 12 |
| 11166 | Microwave-assisted one-pot functionalization of metal-organic framework MIL-53(Al)-NH ₂ with copper(II) complexes and its application in olefin oxidation. <i>Catalysis Science and Technology</i> , 2017, 7, 6069-6079. | 2.1 | 36 |
| 11167 | Triplet Ground-State-Bridged Photochemical Process: Understanding the Photoinduced Chiral Inversion at the Metal Center of [Ru(phen) ₂ (I-ser)] ⁺ and Its Bipy Analogues. <i>Inorganic Chemistry</i> , 2017, 56, 14467-14476. | 1.9 | 7 |
| 11168 | Influence of Relativistic Effects on Bonding Modes in M(II) Dinuclear Complexes (M = Au, Ag, and Cu). <i>Inorganic Chemistry</i> , 2017, 56, 14624-14631. | 1.9 | 21 |
| 11169 | Localized Intrinsic Valence Virtual Orbitals as a Tool for the Automatic Classification of Core Excited States. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5984-5999. | 2.3 | 9 |
| 11170 | Dicationic Thiolate-Bridged Diruthenium Complexes for Catalytic Oxidation of Molecular Dihydrogen. <i>Organometallics</i> , 2017, 36, 4499-4506. | 1.1 | 6 |
| 11171 | Design of superhalogens using a core-shell structure model. <i>Nanoscale</i> , 2017, 9, 18781-18787. | 2.8 | 12 |
| 11172 | Structure-reactivity correlations of the abnormal Beckmann reaction of dihydrolevoglucosenone oxime. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 10105-10115. | 1.5 | 11 |
| 11173 | The Polarization of Polycyclic Aromatic Hydrocarbons Curved by Pentagon Incorporation: The Role of the Flexoelectric Dipole. <i>Journal of Physical Chemistry C</i> , 2017, 121, 27154-27163. | 1.5 | 48 |
| 11174 | Computational modelling of the redistribution of copper isotopes by proteins in the liver. <i>Metallomics</i> , 2017, 9, 1809-1819. | 1.0 | 20 |
| 11176 | Theoretical investigation on the selectivity in the palladium-catalyzed reaction of oxidative carbonylation-carbocyclization-carbonylation-alkynylation of enallene. <i>Journal of Organometallic Chemistry</i> , 2017, 853, 143-148. | 0.8 | 6 |
| 11177 | Self-consistent determination of the fictitious temperature in thermally-assisted-occupation density functional theory. <i>RSC Advances</i> , 2017, 7, 50496-50507. | 1.7 | 33 |
| 11178 | Theoretical Studies of the Glycosidation of 2-O-Substituted 5-Fluorouracil: N-Regioselective Synthesis with the Phase-Transfer-Catalysis Method. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8866-8883. | 1.1 | 4 |
| 11179 | The regioselectivity in the platinum-catalyzed domino reaction to access alkynylated indoles: a theoretical study. <i>New Journal of Chemistry</i> , 2017, 41, 13798-13803. | 1.4 | 2 |
| 11180 | How Well Can the M06 Suite of Functionals Describe the Electron Densities of Ne, Ne ⁶⁺ , and Ne ⁸⁺ ?. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6068-6077. | 2.3 | 25 |
| 11181 | A Theoretical and Computational Analysis of the Methyl-Vinyl + O ₂ Reaction and Its Effects on Propene Combustion. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9173-9184. | 1.1 | 23 |
| 11182 | Theoretical study on the reaction mechanism of ϵ -Ni-catalyzed hydrodesulfurization of aryl sulfide. <i>RSC Advances</i> , 2017, 7, 51475-51484. | 1.7 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11183 | Toward reliable modeling of S-nitrosothiol chemistry: Structure and properties of methyl thionitrite (CH ₃ SNO), an S-nitrosocysteine model. <i>Journal of Chemical Physics</i> , 2017, 147, 044305. | 1.2 | 11 |
| 11184 | First example of crystal structure of the nitrosoruthenium(II) trinitrato complex. <i>Journal of Structural Chemistry</i> , 2017, 58, 975-982. | 0.3 | 4 |
| 11185 | Simultaneous Speciation, Structure, and Equilibrium Constant Determination in the Ni ²⁺ –EDTA–CN [–] Ternary System via High-Resolution Laboratory X-ray Absorption Fine Structure Spectroscopy and Theoretical Calculations. <i>Inorganic Chemistry</i> , 2017, 56, 14220-14226. | 1.9 | 9 |
| 11186 | Use of Low-Cost Quantum Chemistry Procedures for Geometry Optimization and Vibrational Frequency Calculations: Determination of Frequency Scale Factors and Application to Reactions of Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6052-6060. | 2.3 | 32 |
| 11187 | Local Noncollinear Spin Analysis. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6101-6107. | 2.3 | 7 |
| 11188 | Floppy molecules as candidates for achieving optoelectronic molecular devices without skeletal rearrangement or bond breaking. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30842-30851. | 1.3 | 13 |
| 11189 | Redox Noninnocent Azo-Aromatic Pincers and Their Iron Complexes. Isolation, Characterization, and Catalytic Alcohol Oxidation. <i>Inorganic Chemistry</i> , 2017, 56, 14084-14100. | 1.9 | 73 |
| 11190 | Resolving Transition Metal Chemical Space: Feature Selection for Machine Learning and Structure–Property Relationships. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8939-8954. | 1.1 | 168 |
| 11191 | Multiconfiguration Pair-Density Functional Theory Is Free From Delocalization Error. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5616-5620. | 2.1 | 31 |
| 11192 | Understanding the Regioselectivity of Aromatic Hydroxylation over Divanadium-Substituted \hat{I}^3 -Keggin Polyoxotungstate. <i>ACS Catalysis</i> , 2017, 7, 8514-8523. | 5.5 | 23 |
| 11193 | Formation and structure of the ferryl [Fe=O] intermediate in the non-haem iron halogenase SyrB2: classical and QM/MM modelling agree. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30107-30119. | 1.3 | 19 |
| 11194 | Methane Adsorption in Zr-Based MOFs: Comparison and Critical Evaluation of Force Fields. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25309-25322. | 1.5 | 34 |
| 11195 | Dependence of the Electrochemical Redox Properties of Fullerenes on Ionic Liquids. <i>Langmuir</i> , 2017, 33, 13468-13479. | 1.6 | 10 |
| 11196 | Coordinatively- and electronically-unsaturated square planar cobalt(III) complexes of a pyridine dianionic pincer ligand. <i>Dalton Transactions</i> , 2017, 46, 16228-16235. | 1.6 | 9 |
| 11197 | Electrochemistry of triphenylstibine-functionalized Fischer carbene complexes of Molybdenum(0). <i>Electrochimica Acta</i> , 2017, 246, 897-907. | 2.6 | 8 |
| 11198 | Modeling Coronene Nanostructures: Analytical Potential, Stable Configurations and Ab Initio Energies. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14330-14338. | 1.5 | 28 |
| 11199 | Theoretical study on electron structure and charge transport properties of tetraazapentacene derivatives. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 76, 535-542. | 1.3 | 3 |
| 11200 | Synthesis, characterization, antimicrobial and theoretical studies of the first main group tris(ephedrinedithiocarbamate) complexes of As(III), Sb(III), Bi(III), Ga(III) and In(III). <i>Polyhedron</i> , 2017, 134, 221-229. | 1.0 | 16 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11201 | Benchmarking the Fundamental Electronic Properties of small TiO ₂ Nanoclusters by <i>i>GW</i> and Coupled Cluster Theory Calculations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3814-3828. | 2.3 | 24 |
| 11202 | X-ray circular dichroism signals: a unique probe of local molecular chirality. <i>Chemical Science</i> , 2017, 8, 5969-5978. | 3.7 | 27 |
| 11203 | Homo- and Heterobinuclear Cu and Pd Complexes with a Bridging Redox-Active Bisguanidino-Substituted Dioxolene Ligand: Electronic Structure and Metal-Ligand Electron Transfer. <i>Chemistry - A European Journal</i> , 2017, 23, 11636-11648. | 1.7 | 19 |
| 11204 | Accuracy of Frequencies Obtained with the Aid of Explicitly Correlated Wave Function Based Methods. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3602-3613. | 2.3 | 6 |
| 11205 | Ionic liquids with thioether motifs as synthetic cationic lipids for gene delivery. <i>Chemical Communications</i> , 2017, 53, 8328-8331. | 2.2 | 14 |
| 11206 | Proton Shuttling and Reaction Paths in Dissociative Electron Attachment to <i>i>o</i> - and <i>i>p</i> -Tetrafluorohydroquinone, an Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5580-5585. | 1.1 | 2 |
| 11207 | Thermally robust: triarylsulfonium ionic liquids stable in air for 90 days at 300 °C. <i>RSC Advances</i> , 2017, 7, 7623-7630. | 1.7 | 23 |
| 11208 | Palladium(<i>ii</i>) in liquid ammonia: an investigation of structural and dynamical properties by applying quantum mechanical charge field molecular dynamics (QMCF-MD). <i>Dalton Transactions</i> , 2017, 46, 9630-9638. | 1.6 | 14 |
| 11209 | Nuclearity dependent solvent contribution to the catechol oxidase activity of novel copper(<i>ii</i>) complexes derived from Mannich-base ligand platforms: synthesis, crystal structure and mechanism. <i>New Journal of Chemistry</i> , 2017, 41, 8586-8597. | 1.4 | 16 |
| 11210 | Impact of side-chain fluorination on photovoltaic properties: fine tuning of the microstructure and energy levels of 2D-conjugated copolymers. <i>Journal of Materials Chemistry A</i> , 2017, 5, 16702-16711. | 5.2 | 20 |
| 11211 | Structure-property relationships in protic ionic liquids: a thermochemical study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19928-19936. | 1.3 | 15 |
| 11212 | Theoretical insights into the nature of synergistic enhancement in bimetallic CoTiAlPO-5 catalysts for ammonia activation. <i>Catalysis Science and Technology</i> , 2017, 7, 3474-3480. | 2.1 | 3 |
| 11213 | Systematic Functional Analysis of Active-Site Residues in <i>i>L</i> -Threonine Dehydrogenase from <i>i>Thermoplasma volcanium</i> . <i>ACS Omega</i> , 2017, 2, 3308-3314. | 1.6 | 3 |
| 11214 | A new tetrapodal 3-hydroxy-4-pyridinone ligand for complexation of 89zirconium for positron emission tomography (PET) imaging. <i>Dalton Transactions</i> , 2017, 46, 9654-9663. | 1.6 | 27 |
| 11215 | Surprising behaviors in the temperature dependent kinetics of diatomic interhalogens with anions and cations. <i>Journal of Chemical Physics</i> , 2017, 146, 214307. | 1.2 | 7 |
| 11216 | Electronic Structure of Edge-Modified Graphene Quantum Dots Interacting with Polyaniline: Vibrational and Optical Properties. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16576-16583. | 1.5 | 21 |
| 11217 | Self-trapped exciton configurations in Beryllium Oxide. <i>Journal of Physics: Conference Series</i> , 2017, 830, 012158. | 0.3 | 0 |
| 11218 | DFT investigations on the conversion of acetylene to undesired vinyl acetylene during vinyl acetate synthesis. <i>Computational and Theoretical Chemistry</i> , 2017, 1115, 253-260. | 1.1 | 11 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11219 | Combined Theoretical and Experimental Studies of Nickel-Catalyzed Cross-Coupling of Methoxyarenes with Arylboronic Esters via C–O Bond Cleavage. <i>Journal of the American Chemical Society</i> , 2017, 139, 10347-10358. | 6.6 | 87 |
| 11220 | Conjugated Trimeric Scaffolds Accessible from Indolyne Cyclotrimerizations: Synthesis, Structures, and Electronic Properties. <i>Journal of the American Chemical Society</i> , 2017, 139, 10447-10455. | 6.6 | 47 |
| 11221 | Facing the challenge of predicting the standard formation enthalpies of n-butyl-phosphate species with ab initio methods. <i>Journal of Chemical Physics</i> , 2017, 146, 244312. | 1.2 | 4 |
| 11222 | Origins of Stereoselectivity of Enamine–Iminium-Activated Nazarov Cyclizations by Vicinal Diamines. <i>Journal of Organic Chemistry</i> , 2017, 82, 8186-8190. | 1.7 | 7 |
| 11223 | Thermodynamic and orbital studies of the reactivity of amidine with phosphoryl chloride and thionyl chloride. <i>Structural Chemistry</i> , 2017, 28, 1953-1958. | 1.0 | 2 |
| 11224 | Combined Experimental and Computational Study on Ruthenium(II)-Catalyzed Reactions of Dienes with Aldehydes and N,N-Dimethylformamide. <i>Journal of Organic Chemistry</i> , 2017, 82, 7964-7973. | 1.7 | 8 |
| 11225 | Experimental and Theoretical Study of Ionic Pair Dissociation in a Lithium Ion–Linear Polyethylenimine–Polyacrylonitrile Blend for Solid Polymer Electrolytes. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6759-6765. | 1.2 | 16 |
| 11226 | Probing Intermolecular Electron Delocalization in Dimer Radical Anions by Vibrational Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2017, 121, 7327-7335. | 1.2 | 18 |
| 11227 | Hydroxyl radical-mediated degradation of diclofenac revisited: a computational approach to assessment of reaction mechanisms and by-products. <i>Environmental Science and Pollution Research</i> , 2017, 24, 18458-18469. | 2.7 | 25 |
| 11228 | Prediction of the Iron-Based Polynuclear Magnetic Superhalogens with Pseudohalogen CN as Ligands. <i>Inorganic Chemistry</i> , 2017, 56, 7928-7935. | 1.9 | 15 |
| 11229 | Local Structures and Heterogeneity of Silica-Supported M(III) Sites Evidenced by EPR, IR, NMR, and Luminescence Spectroscopies. <i>Journal of the American Chemical Society</i> , 2017, 139, 8855-8867. | 6.6 | 58 |
| 11230 | Unravelling the electronic structure and dynamics of an isolated molecular rotary motor in the gas-phase. <i>Chemical Science</i> , 2017, 8, 6141-6148. | 3.7 | 13 |
| 11231 | Synthesis and detailed conformational analysis of new naphthoxazino[2,3-a]benz[c]azepine and naphthoxazino[2,3-a]thieno[3,2-c]pyridine derivatives. <i>Tetrahedron</i> , 2017, 73, 4790-4804. | 1.0 | 11 |
| 11232 | The application of TD-DFT to excited states of a family of TPD molecules interesting for optoelectronic use. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1. | 0.5 | 2 |
| 11233 | The [3+2] cycloaddition reaction in CpRu(allyl)(acetylene). <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1. | 0.5 | 0 |
| 11234 | Understanding the Lewis Acidity of Co(II) Sites on a Silica Surface. <i>Inorganic Chemistry</i> , 2017, 56, 7731-7736. | 1.9 | 13 |
| 11235 | NLOphoric donor-rigidified ESIPT dyes – Synthesis, pH study, solvatochromism and DFT insights. <i>Journal of Luminescence</i> , 2017, 192, 343-358. | 1.5 | 9 |
| 11236 | Communication: DFT treatment of strong correlation in 3d transition-metal diatomics. <i>Journal of Chemical Physics</i> , 2017, 146, 211105. | 1.2 | 42 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11237 | Effective empirical corrections for basis set superposition error in the def2-SVPD basis: gCP and DFT-C. <i>Journal of Chemical Physics</i> , 2017, 146, 234105. | 1.2 | 39 |
| 11238 | Influences of pressure on methyl group, elasticity, sound velocity and sensitivity of solid nitromethane. <i>European Physical Journal B</i> , 2017, 90, 1. | 0.6 | 14 |
| 11239 | Design, synthesis and multitarget biological profiling of second-generation anti-Alzheimer rhinâ€“huprine hybrids. <i>Future Medicinal Chemistry</i> , 2017, 9, 965-981. | 1.1 | 40 |
| 11240 | Relative stability of 1-(4-R-2,6-dinitrophenyl)-2,2-diphenylhydrazides. <i>Russian Journal of Organic Chemistry</i> , 2017, 53, 679-685. | 0.3 | 3 |
| 11241 | Reaction of 1,5-diphenyl-3-arylverdazyles with Ð;Ð•acids. <i>Russian Journal of Organic Chemistry</i> , 2017, 53, 764-768. | 0.3 | 3 |
| 11242 | Hydrogen bonding characterization in water and small molecules. <i>Journal of Chemical Physics</i> , 2017, 146, 244315. | 1.2 | 8 |
| 11243 | Crystal Structure of the DFNKF Segment of Human Calcitonin Unveils Aromatic Interactions between Phenylalanines. <i>Chemistry - A European Journal</i> , 2017, 23, 2051-2058. | 1.7 | 28 |
| 11244 | Electrical conductivity of dithiophene-based diblock molecular junctions. <i>Computational and Theoretical Chemistry</i> , 2017, 1099, 64-74. | 1.1 | 2 |
| 11245 | Investigation of two o-hydroxy Schiff bases in terms of prototropy and radical scavenging activity. <i>Journal of Molecular Structure</i> , 2017, 1130, 623-632. | 1.8 | 22 |
| 11246 | The quest for best suited references for configuration interaction singles calculations of core excited states. <i>Journal of Computational Chemistry</i> , 2017, 38, 116-126. | 1.5 | 12 |
| 11247 | A systematic study of ²⁵ Mg NMR in paramagnetic transition metal oxides: applications to Mg-ion battery materials. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 613-625. | 1.3 | 50 |
| 11248 | Zinc Complexes of Cyclodextrinâ€“bearing 8â€“Hydroxyquinoline Ligands: A Comparative Study. <i>Chemistry - an Asian Journal</i> , 2017, 12, 110-115. | 1.7 | 15 |
| 11249 | Mechanistic investigation into Et ₃ N C-H activation and chemoselectivity by Pd-Catalyzed intramolecular heck reaction of N-Vinylacetamides. <i>Journal of Organometallic Chemistry</i> , 2017, 827, 56-66. | 0.8 | 15 |
| 11250 | Charge-transfer contributions to the excitonic coupling matrix element in BODIPY-based energy transfer cassettes. <i>Chemical Physics</i> , 2017, 482, 265-276. | 0.9 | 16 |
| 11251 | The thermochromic behavior of aromatic amine-SO ₂ charge transfer complexes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 173, 462-467. | 2.0 | 11 |
| 11252 | How reliable is DFT in predicting relative energies of polycyclic aromatic hydrocarbon isomers? comparison of functionals from different rungs of Jacob's ladder. <i>Journal of Computational Chemistry</i> , 2017, 38, 370-382. | 1.5 | 43 |
| 11253 | Electron localization function from density components. <i>Journal of Computational Chemistry</i> , 2017, 38, 204-210. | 1.5 | 19 |
| 11254 | Stability of the chlorinated derivatives of the DNA/RNA nucleobases, purine and pyrimidine toward radical formation via homolytic C-Cl bond dissociation. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25319. | 1.0 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11255 | Open-ended formulation of self-consistent field response theory with the polarizable continuum model for solvation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 366-379. | 1.3 | 5 |
| 11256 | Coordination to Imidazole Ring Switches on Phosphorescence of Platinum Cyclometalated Complexes: The Route to Selective Labeling of Peptides and Proteins via Histidine Residues. <i>Bioconjugate Chemistry</i> , 2017, 28, 426-437. | 1.8 | 25 |
| 11257 | Novel Thiazole Based Styryl Dyes with Benzimidazole Unit - Synthesis, Photophysical and TD-DFT Studies. <i>Journal of Fluorescence</i> , 2017, 27, 167-180. | 1.3 | 8 |
| 11258 | Structural characterization of phosphatidylglycerol model membranes containing the antibiotic target lipid II molecule: a Raman microspectroscopy study. <i>Journal of Raman Spectroscopy</i> , 2017, 48, 170-179. | 1.2 | 8 |
| 11259 | Green fluorescent protein chromophore derivatives as a new class of aldose reductase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2017, 125, 965-974. | 2.6 | 12 |
| 11260 | Raman spectroscopy study on influence of network architecture on hydration of poly(2-(2-methoxyethoxy)ethyl methacrylate) hydrogels. <i>Journal of Raman Spectroscopy</i> , 2017, 48, 465-473. | 1.2 | 21 |
| 11261 | Isomeric effects on the self-assembly of a plausible prebiotic nucleoside analogue: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2017, 117, 213-221. | 1.0 | 2 |
| 11262 | Spectroscopic Properties of Amine-substituted Analogues of Firefly Luciferin and Oxyluciferin. <i>Photochemistry and Photobiology</i> , 2017, 93, 486-494. | 1.3 | 19 |
| 11263 | Dynamics of NH ₃ ligands and ClO ₄ ⁻ anions in the phase transition in [Cd(NH ₃) ₆](ClO ₄) ₂ studied by x-ray powder diffraction, neutron scattering methods and infrared spectroscopy. <i>Journal of Physics and Chemistry of Solids</i> , 2017, 101, 34-44. | 1.9 | 0 |
| 11264 | Molecular modeling, dynamics studies and density functional theory approaches to identify potential inhibitors of SIRT4 protein from <i>Homo sapiens</i> : a novel target for the treatment of type 2 diabetes. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 3316-3329. | 2.0 | 39 |
| 11265 | Fe-Li Interactions in Ferrocenyllithium Compounds. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 483-488. | 1.0 | 3 |
| 11266 | Theoretical study of fragmentation pathways and product distribution of deprotonated aspartic acid. <i>Computational and Theoretical Chemistry</i> , 2017, 1099, 1-7. | 1.1 | 2 |
| 11267 | Reactivity of contact ion pairs in a charged monotopic receptor. <i>International Journal of Mass Spectrometry</i> , 2017, 418, 198-203. | 0.7 | 2 |
| 11268 | Pt(II) nitrile complexes: New insights on old complexes from a combined experimental and theoretical study. <i>Inorganica Chimica Acta</i> , 2017, 455, 489-504. | 1.2 | 6 |
| 11269 | Experimental and quantum chemical studies on the molecular structure of 3,3,3-trifluoropropane-1-sulfonyl chloride: CF ₃ CH ₂ CH ₂ SO ₂ Cl. <i>Journal of Molecular Structure</i> , 2017, 1127, 377-385. | 1.8 | 1 |
| 11270 | Synthesis, crystal structure and luminescence properties of acenaphthene benzohydrazide based ligand and its zinc(II) complex. <i>Journal of Molecular Structure</i> , 2017, 1128, 195-204. | 1.8 | 22 |
| 11271 | X-ray crystal structure, infrared, Raman and density functional studies of 7-azaindole-3-carboxaldehyde. <i>Journal of Molecular Structure</i> , 2017, 1128, 186-194. | 1.8 | 8 |
| 11272 | Enhancing glycan isomer separations with metal ions and positive and negative polarity ion mobility spectrometry-mass spectrometry analyses. <i>Analytical and Bioanalytical Chemistry</i> , 2017, 409, 467-476. | 1.9 | 78 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11273 | Insight into opto-electronic property by modifying optical layers with multi-polar and multi-branched structures. <i>Journal of Materials Science: Materials in Electronics</i> , 2017, 28, 1489-1500. | 1.1 | 4 |
| 11274 | Aggregates of diketopyrrolopyrrole dimers in solution. <i>Dyes and Pigments</i> , 2017, 136, 678-685. | 2.0 | 13 |
| 11275 | Diaminomaleonitrile-based azo receptors: Synthesis, DFT studies and their antibacterial activities. <i>Journal of Molecular Structure</i> , 2017, 1129, 169-178. | 1.8 | 12 |
| 11276 | Main-chain alternating fullerene and dye oligomers for organic photovoltaics. <i>Polymer International</i> , 2017, 66, 388-398. | 1.6 | 11 |
| 11277 | Donor- and acceptor-functionalized dibenzo[a,e]pentalenes: modulation of the electronic band gap. <i>Organic Chemistry Frontiers</i> , 2017, 4, 658-663. | 2.3 | 39 |
| 11278 | Thermochemistry of 4-HOC ₆ H ₄ COR (R = H, CH ₃ , C ₂ H ₅ , n-C ₃ H ₇ , n-C ₄ H ₉ , n-C ₅ H ₁₁ , and n-C ₆ H ₁₃) Tj ETOq1 1 0,784314 | 1.0 | 9 |
| 11279 | Infrared spectral evidence and DFT calculations of hydrogen-bonding and molecular structures of acetogenins. <i>Journal of Molecular Structure</i> , 2017, 1130, 174-180. | 1.8 | 4 |
| 11280 | Structures and spectroscopic properties of sulfur-nitrogen-pnictogen chains: R ₂ Pâ€“N S Nâ€“PR ₂ and R ₂ Pâ€“N S Nâ€“AsR ₂ . <i>Journal of Molecular Structure</i> , 2017, 1132, 102-108. | 1.8 | 0 |
| 11281 | Molecular structure, spectroscopic (FT-IR, FT Raman, UV, NMR and THz) investigation and hyperpolarizability studies of 3-(2-Chloro-6-fluorophenyl)-1-(2-thienyl) prop-2-en-1-one. <i>Journal of Molecular Structure</i> , 2017, 1129, 292-304. | 1.8 | 35 |
| 11282 | The Magnetic Transition of Tcn (n=1, 2) Induced by the Reaction with Cl and BO ₂ . <i>Journal of Cluster Science</i> , 2017, 28, 905-915. | 1.7 | 0 |
| 11283 | Conformational properties of 1-cyano-1-silacyclohexane, C ₅ H ₁₀ SiHCN: Gas electron diffraction, low-temperature NMR and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2017, 1132, 149-156. | 1.8 | 11 |
| 11284 | Conformational stability, spectral analysis (infrared, Raman and NMR) and DFT calculations of 2-Amino-5-(ethylthio)-1,3,4-thiadiazole. <i>Journal of Molecular Structure</i> , 2017, 1130, 434-441. | 1.8 | 13 |
| 11285 | Preparation of 3-(9-Anthryl)acrylates and 9-Aroylethenylantracenes as Pi-Extended Anthracenes and Their Dielsâ€“Alder Type Adducts with Electron-Poor Dienophiles. <i>Polycyclic Aromatic Compounds</i> , 2017, 37, 148-160. | 1.4 | 2 |
| 11286 | Copper(I)-catalyzed reaction of unsymmetrical alkyne with HB(<sc>pin</sc>): a density functional theory study. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3630. | 0.9 | 3 |
| 11287 | Mechanistic study on silver(I)-catalyzed aminofluorination of unactivated alkenes. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3655. | 0.9 | 7 |
| 11288 | Are there reliable DFT approaches for ¹³ C NMR chemical shift predictions of fullerene C ₆₀ derivatives?. <i>International Journal of Quantum Chemistry</i> , 2017, 117, 7-14. | 1.0 | 11 |
| 11289 | Substitution of Metallocenes with [2.2]Paracyclophane to Enable Confocal Microscopy Imaging in Living Cells. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 297-305. | 1.0 | 13 |
| 11290 | Contribution of trans -aconitic acid to DPPH scavenging ability in different media. <i>Food Chemistry</i> , 2017, 214, 447-452. | 4.2 | 23 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11291 | Study of vibrational spectra and hydrogen bonding network in dimeric and tetrameric model of ampicillin using DFT and AIM approach. <i>Journal of Molecular Structure</i> , 2017, 1131, 225-235. | 1.8 | 11 |
| 11292 | Radical degradation stability of ether linkage in N,N,N',N'-tetraoctyldiglycolamide and related organic extractants: A density functional study. <i>Progress in Nuclear Energy</i> , 2017, 94, 208-215. | 1.3 | 12 |
| 11293 | Viability of dodecahedrane-forming radical polycyclizations. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 1976-1979. | 1.5 | 4 |
| 11294 | Theoretical study on the phenylpropanolamine drug interaction with the pristine, Si and Al doped [60] fullerenes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2017, 87, 186-191. | 1.3 | 33 |
| 11295 | Triammine <i>fac</i> and <i>mer</i> Coordination for Ruthenium Nitrosyl Complexes: Synthesis and Characterization of $[\text{RuNO}(\text{NH}_3)_3\text{Cl}_2]\text{Cl}$. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 971-978. | 1.0 | 9 |
| 11296 | Molybdenum(0) Fischer ethoxycarbene complexes: Synthesis, X-ray crystal structures and DFT study. <i>Polyhedron</i> , 2017, 121, 285-296. | 1.0 | 6 |
| 11297 | The crystal structure of carbamoyl fluoride, NH_2COF . <i>Structural Chemistry</i> , 2017, 28, 303-307. | 1.0 | 5 |
| 11298 | Modulating hydrogen-bond basicity within the context of protein-ligand binding: A case study with thrombin inhibitors that reveals a dominating role for desolvation. <i>European Journal of Medicinal Chemistry</i> , 2017, 125, 975-991. | 2.6 | 6 |
| 11299 | A new structural arrangement in proteins involving lysine NH_3^+ group and carbonyl. <i>Scientific Reports</i> , 2017, 7, 16402. | 1.6 | 10 |
| 11300 | A luminescent bis(pyridyl)-substituted benzimidazole platinum(II) complex exhibiting an intermolecular anagostic interaction. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2017, 73, 697-702. | 0.2 | 2 |
| 11301 | Exploring dissociative water adsorption on isoelectronically BN doped graphene using alchemical derivatives. <i>Journal of Chemical Physics</i> , 2017, 147, 164113. | 1.2 | 25 |
| 11302 | Infrared absorption spectra of partially deuterated methoxy radicals CH_2DO and CHD_2O isolated in solid <i>para</i> -hydrogen. <i>Journal of Chemical Physics</i> , 2017, 147, 154305. | 1.2 | 16 |
| 11303 | Zeroth order regular approximation approach to electric dipole moment interactions of the electron. <i>Journal of Chemical Physics</i> , 2017, 147, 014109. | 1.2 | 16 |
| 11304 | Identifying the structure of 4-chlorophenyl isocyanide adsorbed on Au(111) and Pt(111) surfaces by first-principles simulations of Raman spectra. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32389-32397. | 1.3 | 12 |
| 11305 | Testing a simple approach for theoretical evaluation of radiolysis products in extraction systems. A case of N,O -donor ligands for Am/Eu separation. <i>RSC Advances</i> , 2017, 7, 55441-55449. | 1.7 | 14 |
| 11306 | Experimental (X-ray, FT-IR, and UV-Vis Spectroscopy) and Theoretical Methods (DFT Study) of N' -(Dipyridin-2-ylmethylene)-4-methylbenzenesulfonohydrazide. <i>Crystallography Reports</i> , 2017, 62, 1122-1127. | 0.1 | 2 |
| 11307 | Tetranuclear Ni_4 and Co_4 Schiff-base complexes with an M_4O_6 defective dicubane-like core: zero-field SMM behavior in the cobalt analogue. <i>New Journal of Chemistry</i> , 2017, 41, 11258-11267. | 1.4 | 34 |
| 11308 | Insights into the structure of triethylammoniumbis(pyridine-2,6-dicarboxylato-iron(III)): Crystallographic and theoretical study. <i>Molecular Crystals and Liquid Crystals</i> , 2017, 658, 140-152. | 0.4 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11309 | Exploring the Interactions of Atomic Oxygen on Silver Clusters with Hydrogen. <i>Chinese Journal of Chemical Physics</i> , 2017, 30, 685-690. | 0.6 | 2 |
| 11310 | Theoretical Evaluation of the Efficiency of Novel Frustrated Lewis Pairs in the <i>cis</i> -Hydrogenation Reaction of Dimethylacetylene. <i>Progress in Reaction Kinetics and Mechanism</i> , 2017, 42, 372-383. | 1.1 | 1 |
| 11311 | Spectroscopic investigation, DFT calculations and cytotoxic activity of a 1-amino-1,3-dihydrospiro[imidazoline-4,2-indene]-2,5-dione and its platinum and palladium complexes. <i>Arkivoc</i> , 2017, 2016, 235-246. | 0.3 | 0 |
| 11312 | Synthesis of Fréchet-type poly(aryl ether) dendrimers with allyl end groups: comparative convergent and divergent approaches. <i>Arkivoc</i> , 2017, 2017, 117-128. | 0.3 | 2 |
| 11313 | Computing Free Energies of Hydroxylated Silica Nanoclusters: Forcefield versus Density Functional Calculations. <i>Inorganics</i> , 2017, 5, 41. | 1.2 | 3 |
| 11314 | DMAP-assisted sulfonylation as an efficient step for the methylation of primary amine motifs on solid support. <i>Beilstein Journal of Organic Chemistry</i> , 2017, 13, 806-816. | 1.3 | 9 |
| 11315 | First-Principles View on Photoelectrochemistry: Water-Splitting as Case Study. <i>Inorganics</i> , 2017, 5, 37. | 1.2 | 22 |
| 11316 | The Silacyclobutene Ring: An Indicator of Triplet State Baird-Aromaticity. <i>Inorganics</i> , 2017, 5, 91. | 1.2 | 5 |
| 11317 | Cytotoxicity and Antioxidant Potential of Novel 2-(2-((1H-indol-5yl)methylene)-hydrazinyl)-thiazole Derivatives. <i>Molecules</i> , 2017, 22, 260. | 1.7 | 45 |
| 11318 | Design, Synthesis and Biological Evaluation of 2-(2-Amino-5(6)-nitro-1H-benzimidazol-1-yl)-N-arylacetamides as Antiprotozoal Agents. <i>Molecules</i> , 2017, 22, 579. | 1.7 | 9 |
| 11319 | A DFT Study of the Geometrical, Spectroscopical and Reactivity Properties of Diindolylmethane-Phenylboronic Acid Hybrids. <i>Molecules</i> , 2017, 22, 1744. | 1.7 | 11 |
| 11320 | A Comprehensive Overview of the DFT-D3 London-Dispersion Correction. , 2017, , 195-219. | | 57 |
| 11321 | In Search of the Reason for the Breathing Effect of MIL53 Metal-Organic Framework: An ab Initio Multiconfigurational Study. <i>Frontiers in Chemistry</i> , 2017, 5, 111. | 1.8 | 10 |
| 11322 | Excitons in Solids from Time-Dependent Density-Functional Theory: Assessing the Tamm-Dancoff Approximation. <i>Computation</i> , 2017, 5, 9. | 1.0 | 12 |
| 11323 | Binuclear Copper(I) Borohydride Complex Containing Bridging Bis(diphenylphosphino) Methane Ligands: Polymorphic Structures of $[(\mu_2\text{-dppm})_2\text{Cu}_2(\text{i-2-BH}_4)_2]$ Dichloromethane Solvate. <i>Crystals</i> , 2017, 7, 318. | 1.0 | 13 |
| 11324 | Distal [FeS]-Cluster Coordination in [NiFe]-Hydrogenase Facilitates Intermolecular Electron Transfer. <i>International Journal of Molecular Sciences</i> , 2017, 18, 100. | 1.8 | 10 |
| 11325 | Switching Activity of Allosteric Modulators Controlled by a Cluster of Residues Forming a Pressure Point in the mGluR5 GPCR. <i>Advances in Quantum Chemistry</i> , 2017, 75, 147-174. | 0.4 | 0 |
| 11326 | Characterization of the Photochemical Properties of 5-Benzyluracil via Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3909-3917. | 1.1 | 15 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11327 | X-Ray Crystallographic Analysis, EPR Studies, and Computational Calculations of a Cu(II) Tetramic Acid Complex. <i>Bioinorganic Chemistry and Applications</i> , 2017, 2017, 1-10. | 1.8 | 4 |
| 11328 | Study of the Molecular Properties of Mono- and Binuclear Metal s-Indacenyl Complexes with Ir, Rh, and Re: A Theoretical Approach. <i>Journal of Chemistry</i> , 2017, 2017, 1-8. | 0.9 | 0 |
| 11329 | Five Regioisomers of Dimethyl Dodecahedrane Derivatives: A Hybrid DFT B3LYP Study. <i>Journal of Chemistry</i> , 2017, 2017, 1-7. | 0.9 | 1 |
| 11330 | Synthesis, Crystal Structure, and DFT Study of Ethyl 1-(2-(Hydroxyimino)-2-phenylethyl)-3-phenyl-1H-pyrazole-5-carboxylate. <i>Journal of Chemistry</i> , 2017, 2017, 1-9. | 0.9 | 4 |
| 11331 | Quantum Chemistry Applied to Photocatalysis with TiO ₂ . , 2017, , . | | 3 |
| 11332 | Triptycene-terminated thiolate and selenolate monolayers on Au(111). <i>Beilstein Journal of Nanotechnology</i> , 2017, 8, 892-905. | 1.5 | 18 |
| 11333 | Transformation of Cadmium Tetracyanoquinodimethane (TCNQ) into a Cadmium Terephthalate Metal-Organic Framework. <i>Australian Journal of Chemistry</i> , 2017, 70, 973. | 0.5 | 1 |
| 11334 | The role of annular nitrogen in tuning the reactivity of bifunctional platinum(II) complexes appended to pyridyl spacers; A kinetic and mechanistic investigation. <i>Journal of Coordination Chemistry</i> , 2017, , 1-20. | 0.8 | 5 |
| 11335 | Quantum Chemical Study of Regularities of Electrophilic Substitution in the Synthesis of Pyrroloquinolines. <i>Moscow University Chemistry Bulletin</i> , 2017, 72, 275-281. | 0.2 | 0 |
| 11336 | Comprehensive investigation of the electronic excitation of W(CO) ₆ by photoabsorption and theoretical analysis in the energy region from 3.9 to 10.8 eV. <i>Beilstein Journal of Nanotechnology</i> , 2017, 8, 2208-2218. | 1.5 | 5 |
| 11337 | Computational Study of Solvation Free Energy, Dipole Moment, Polarizability, Hyperpolarizability and Molecular Properties of Betulin, a Constituent of <i>Corypha taliera</i> (Roxb.). <i>Dhaka University Journal of Pharmaceutical Sciences</i> , 2017, 16, 1-9. | 0.1 | 7 |
| 11338 | Infrared Investigations of the Neutral-Ionic Phase Transition in TTF-CA and Its Dynamics. <i>Crystals</i> , 2017, 7, 17. | 1.0 | 15 |
| 11339 | Wavefunction Theory Approaches to Noncovalent Interactions. , 2017, , 137-168. | | 4 |
| 11340 | Insights into Molecular Beryllium-Silicon Bonds. <i>Inorganics</i> , 2017, 5, 22. | 1.2 | 6 |
| 11341 | Experimental and Theoretical Study of Ketoconazole as Corrosion Inhibitor for Bronze in NaCl+Na ₂ SO ₄ Solution. <i>International Journal of Electrochemical Science</i> , 2017, , 11428-11445. | 0.5 | 12 |
| 11342 | Reduction potential tuning of first row transition metal MIII/MII (M = Cr, Mn, Fe, Co, Ni) hexadentate complexes for viable aqueous redox flow battery catholytes: A DFT study. <i>Electrochimica Acta</i> , 2017, 246, 156-164. | 2.6 | 8 |
| 11343 | Targeting ideal acceptor-donor materials based on hexabenzocoronene. <i>Journal of Molecular Structure</i> , 2018, 1161, 442-452. | 1.8 | 5 |
| 11344 | Glycoconjugate Oxime Formation Catalyzed at Neutral pH: Mechanistic Insights and Applications of 1,4-Diaminobenzene as a Superior Catalyst for Complex Carbohydrates. <i>Bioconjugate Chemistry</i> , 2018, 29, 1219-1230. | 1.8 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11345 | The Effect of Pyrazolyl Substituents on the Photophysical and Photochemical Properties of Pyrazine Derivatives. <i>Photochemistry and Photobiology</i> , 2018, 94, 845-852. | 1.3 | 8 |
| 11346 | Electronic structure and optical properties of boron difluoride naphthaloyl- and anthracenoylacetates. <i>Journal of Luminescence</i> , 2018, 195, 79-86. | 1.5 | 9 |
| 11347 | Machine Learning of Partial Charges Derived from High-Quality Quantum-Mechanical Calculations. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 579-590. | 2.5 | 117 |
| 11348 | NMR spin-spin coupling constants in hydrogen-bonded glycine clusters. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25608. | 1.0 | 4 |
| 11349 | Theoretical study of chromophores for biological sensing: Understanding the mechanism of rhodol based multi-chromophoric systems. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 198, 123-135. | 2.0 | 1 |
| 11350 | An Iron Complex with a Bent, O-coordinated CO ₂ Ligand Discovered by Femtosecond Mid-Infrared Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 5000-5005. | 7.2 | 20 |
| 11351 | Theoretical calculation of NMR shifts in newly developed antibacterial 4-formylbenzoic acid-based thiazoles. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1. | 0.5 | 4 |
| 11352 | Insight into the Electrochemical Reduction Mechanism of Pt(IV) Anticancer Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 3411-3419. | 1.9 | 33 |
| 11353 | Elucidating the Solution-Phase Structure and Behavior of 8-Hydroxyquinoline Zinc in DMSO. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2906-2914. | 1.1 | 4 |
| 11354 | Enhancing Cooperativity in Bifunctional Acid-Pd Catalysts with Carboxylic Acid-Functionalized Organic Monolayers. <i>Journal of Physical Chemistry C</i> , 2018, 122, 6637-6647. | 1.5 | 22 |
| 11355 | A meta-GGA level screened range-separated hybrid functional by employing short range Hartree-Fock with a long range semilocal functional. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8999-9005. | 1.3 | 21 |
| 11356 | An Iron Complex with a Bent, O-coordinated CO ₂ Ligand Discovered by Femtosecond Mid-Infrared Spectroscopy. <i>Angewandte Chemie</i> , 2018, 130, 5094-5099. | 1.6 | 9 |
| 11357 | Nature of bonding and cooperativity in linear DMSO clusters: A DFT, AIM and NCI analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 81, 50-59. | 1.3 | 58 |
| 11358 | Predicting Productive Binding Modes for Substrates and Carbocation Intermediates in Terpene Synthases-Bornyl Diphosphate Synthase As a Representative Case. <i>ACS Catalysis</i> , 2018, 8, 3322-3330. | 5.5 | 34 |
| 11359 | Theoretical insight into the zinc(ii)-catalyzed synthesis of 2-indolyltetrahydroquinolines from N-propargylanilines and indoles: cross-dehydrogenative coupling with temporally separated catalytic activity. <i>Catalysis Science and Technology</i> , 2018, 8, 1997-2007. | 2.1 | 2 |
| 11360 | Salen-indium/triarylborane triads: synthesis and ratiometric emission-colour changes by fluoride ion binding. <i>Dalton Transactions</i> , 2018, 47, 5310-5317. | 1.6 | 13 |
| 11361 | The multichannel <i>i</i> -propyl + O ₂ reaction surface: Definitive theory on a model hydrocarbon oxidation mechanism. <i>Journal of Chemical Physics</i> , 2018, 148, . | 1.2 | 14 |
| 11362 | Properties of C ₄ F ₇ N-CO ₂ thermal plasmas: thermodynamic properties, transport coefficients and emission coefficients. <i>Journal Physics D: Applied Physics</i> , 2018, 51, 155206. | 1.3 | 59 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11363 | Li ₂ B ₁₂ and Li ₃ B ₁₂ : Prediction of the Smallest Tubular and Cage-like Boron Structures. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 4627-4631. | 7.2 | 73 |
| 11364 | Mechanistic insights into asymmetric reductive coupling of isoquinolines by a chiral diboron with DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 97-104. | 0.8 | 13 |
| 11365 | Prediction of ¹⁹ F NMR Chemical Shifts for Fluorinated Aromatic Compounds. <i>Journal of Organic Chemistry</i> , 2018, 83, 3220-3225. | 1.7 | 31 |
| 11366 | Hyper Open-Shell Excited Spin States of Transition-Metal Compounds: FeF ₂ , FeF ₂ ·Ethane, and FeF ₂ ·Ethylene. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2563-2579. | 1.1 | 12 |
| 11367 | Contrasting Transport and Electrostatic Properties of Selectively Fluorinated Alkanethiol Monolayers with Embedded Dipoles. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4881-4890. | 1.5 | 13 |
| 11368 | Energy vs. density on paths toward more exact density functionals. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7538-7548. | 1.3 | 18 |
| 11369 | Elucidating the Nature of the Excited State of a Heteroleptic Copper Photosensitizer by using Time-Resolved X-ray Absorption Spectroscopy. <i>Chemistry - A European Journal</i> , 2018, 24, 6464-6472. | 1.7 | 34 |
| 11370 | Density functional theory calculations of the non-resonant and resonant X-ray emission spectroscopy of carbon fullerenes and nanotubes. <i>Chemical Physics Letters</i> , 2018, 696, 119-124. | 1.2 | 10 |
| 11371 | Time-dependent broken-symmetry density functional theory simulation of the optical response of entangled paramagnetic defects: Color centers in lithium fluoride. <i>Physical Review B</i> , 2018, 97, . | 1.1 | 3 |
| 11372 | The NASA Ames PAH IR Spectroscopic Database: Computational Version 3.00 with Updated Content and the Introduction of Multiple Scaling Factors. <i>Astrophysical Journal, Supplement Series</i> , 2018, 234, 32. | 3.0 | 109 |
| 11373 | Mixed salt of sarcosine containing dimeric undecafluorodialuminate anion and fluoride ion. <i>Journal of Fluorine Chemistry</i> , 2018, 209, 73-78. | 0.9 | 2 |
| 11374 | Structure and Dynamics of Zr ₆ O ₈ Metal-Organic Framework Node Surfaces Probed with Ethanol Dehydration as a Catalytic Test Reaction. <i>Journal of the American Chemical Society</i> , 2018, 140, 3751-3759. | 6.6 | 150 |
| 11375 | Li ₂ B ₁₂ and Li ₃ B ₁₂ : Prediction of the Smallest Tubular and Cage-like Boron Structures. <i>Angewandte Chemie</i> , 2018, 130, 4717-4721. | 1.6 | 8 |
| 11376 | Modification of Gold's Work Function upon Adsorption of Mercaptobiphenylcarbonitrile: Experimental Evidence for a Theoretical Prediction. <i>Journal of Physical Chemistry C</i> , 2018, 122, 6083-6092. | 1.5 | 4 |
| 11377 | Towards reliable references for electron paramagnetic resonance parameters based on quantum chemistry: the case of verdazyl radicals. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7661-7675. | 1.3 | 8 |
| 11378 | Automated error control in divide-and-conquer self-consistent field calculations. <i>Journal of Computational Chemistry</i> , 2018, 39, 909-916. | 1.5 | 11 |
| 11379 | Bridging the Gap between Pentacene and Perfluoropentacene: Synthesis and Characterization of 2,3,9,10-Tetrafluoropentacene in the Neutral, Cationic, and Dicationic States. <i>Journal of Organic Chemistry</i> , 2018, 83, 3149-3158. | 1.7 | 24 |
| 11380 | Infrared Spectroscopy of Matrix-Isolated Neutral and Ionized Anthracoronene in Argon. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2361-2375. | 1.1 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11381 | Exploring Nuclear Photorelaxation of Pyranine in Aqueous Solution: an Integrated Ab-Initio Molecular Dynamics and Time Resolved Vibrational Analysis Approach. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2884-2893. | 1.1 | 29 |
| 11382 | On the contribution of f electrons to the quadratic hyperpolarizability: the case of lanthanide terpyridyl complexes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7401-7406. | 1.3 | 2 |
| 11383 | Understanding and Controlling the Dielectric Response of Metal-Organic Frameworks. <i>ChemPlusChem</i> , 2018, 83, 308-316. | 1.3 | 36 |
| 11384 | Highly accurate equilibrium structure of the C _{2h} symmetric N1- π -CO ₂ hydrogen-bonded uracil-dimer. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25624. | 1.0 | 8 |
| 11385 | Twisted Intramolecular Charge Transfer States in Trinary Star-Shaped Triphenylamine-Based Compounds. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3218-3226. | 1.1 | 29 |
| 11386 | Insight into catalytic reduction of CO ₂ to methane with silanes using Brookhart's cationic Ir(pincer) pincer complex. <i>RSC Advances</i> , 2018, 8, 9232-9242. | 1.7 | 11 |
| 11387 | Synthesis of an unusual quinazoline alkaloid: theoretical and experimental investigations of its structural, electronic, molecular and biological properties. <i>RSC Advances</i> , 2018, 8, 8259-8268. | 1.7 | 21 |
| 11388 | Influence of ligand-bridged substitution on the exchange coupling constant of chromium-wheels host complexes: a density functional theory study. <i>Molecular Physics</i> , 2018, 116, 1306-1319. | 0.8 | 2 |
| 11389 | Mechanistic insights into the selective hydrogenation of resorcinol to 1,3-cyclohexanedione over Pd/rGO catalyst through DFT calculation. <i>Chinese Journal of Chemical Engineering</i> , 2018, 26, 2542-2548. | 1.7 | 6 |
| 11390 | Assessment of Fragmentation Strategies for Large Proteins Using the Multilayer Molecules-in-Molecules Approach. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1383-1394. | 2.3 | 29 |
| 11391 | Computational mechanistic study of Ru-catalyzed CO ₂ reduction by pinacolborane revealing the σ -C-C coupling mechanism for CO ₂ decarbonylation. <i>Dalton Transactions</i> , 2018, 47, 4804-4819. | 1.6 | 6 |
| 11392 | Effective computational route towards vibrational optical activity spectra of chiral molecules in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 9181-9197. | 1.3 | 46 |
| 11393 | Combined Experimental and Computational Study on Catalytic Cyclocoupling of Epoxides and CO ₂ Using Porphyrin-Based Cu(II) Metal-Organic Frameworks with 2D Coordination Networks. <i>Bulletin of the Chemical Society of Japan</i> , 2018, 91, 383-390. | 2.0 | 5 |
| 11394 | Solution Structure and Ultrafast Vibrational Relaxation of the PtPOP Complex Revealed by μ -SCF-QM/MM Direct Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 7100-7119. | 1.5 | 46 |
| 11395 | C-H Alkynylation of N-Methylisoquinolone by Rhodium or Gold Catalysis: Theoretical Studies on the Mechanism, Regioselectivity, and Role of TIPS-EBX. <i>Organometallics</i> , 2018, 37, 1026-1033. | 1.1 | 16 |
| 11396 | Intramolecular stabilization of a catalytic [FeFe]-hydrogenase mimic investigated by experiment and theory. <i>Dalton Transactions</i> , 2018, 47, 4941-4949. | 1.6 | 16 |
| 11397 | High-resolution photoelectron spectroscopy of TiO ₃ H ₂ ²⁻ : Probing the TiO ₂ ²⁻ + H ₂ O dissociative adduct. <i>Journal of Chemical Physics</i> , 2018, 148, 222810. | 1.2 | 20 |
| 11398 | A Maze of Dyotropic Rearrangements and Triple Shifts: Carbocation Rearrangements Connecting Stemarene, Stomodene, Betaerdene, Aphidicolene, and Scopadulanol. <i>Journal of Organic Chemistry</i> , 2018, 83, 3780-3793. | 1.7 | 16 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11399 | Triplet state homoaromaticity: concept, computational validation and experimental relevance. <i>Chemical Science</i> , 2018, 9, 3165-3176. | 3.7 | 16 |
| 11400 | Projection-Based Correlated Wave Function in Density Functional Theory Embedding for Periodic Systems. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1928-1942. | 2.3 | 70 |
| 11401 | Computational prediction of chemical reactions: current status and outlook. <i>Drug Discovery Today</i> , 2018, 23, 1203-1218. | 3.2 | 126 |
| 11402 | Structure-fluorescence relationship of push-pull 2-phenylbenzothiazole derivatives designed based on the firefly light-emitter. <i>Tetrahedron Letters</i> , 2018, 59, 1431-1434. | 0.7 | 4 |
| 11403 | QM/MM reveals the sequence of substrate binding during OPRT action. <i>Computational Biology and Chemistry</i> , 2018, 74, 31-38. | 1.1 | 4 |
| 11404 | Theoretical exploration on switchable NLO response induced by redox properties of polyoxometalates [XNbW ₁₁ O ₄₀] ⁿ⁻ /(n+1)- (X = Al, Si, P, S, Ga, Ge, As, Se). <i>Journal of Molecular Graphics and Modelling</i> , 2018, 81, 155-161. | 1.3 | 1 |
| 11405 | B-phenylated o-carboranes and its chromium derivatives: Synthesis, electrochemical properties, and X-ray structural studies. <i>Journal of Organometallic Chemistry</i> , 2018, 865, 100-108. | 0.8 | 3 |
| 11406 | Reduced Graphene oxide / Nanoparticle hybrid structures: A new generation smart materials for optical sensors. <i>Materials Today: Proceedings</i> , 2018, 5, 2609-2618. | 0.9 | 6 |
| 11407 | Conformational dynamics of 4-formylaminoantipyrene based on NMR and theoretical calculations. <i>Journal of Molecular Structure</i> , 2018, 1163, 280-286. | 1.8 | 3 |
| 11408 | Theoretical Study of the Oxidation of Methane to Methanol by the [CuII CuI(1/4-O)2CuIII(7-N-Etppz)] ¹⁺ Complex. <i>Inorganic Chemistry</i> , 2018, 57, 3261-3271. | 1.9 | 9 |
| 11409 | Computational and Spectroscopic Analysis of 1 ² -Indandione Modified Zinc Porphyrins. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4448-4456. | 1.1 | 6 |
| 11410 | Dipolar Relaxation in Functionalized Poly- <i>p</i> -phenylenes Bearing Ultrastrong Dipoles Perpendicular to the Backbone. <i>Macromolecules</i> , 2018, 51, 3330-3339. | 2.2 | 1 |
| 11411 | Viscosity induced emission of red-emitting NLOphoric coumarin morpholine-thiazole hybrid styryl dyes as FMRs: Consolidated experimental and theoretical approach. <i>Optical Materials</i> , 2018, 79, 90-107. | 1.7 | 16 |
| 11412 | Experimental and theoretical research on 1 ³ -irradiated 7-methoxy-4-methylcoumarin powder through EPR and DFT methods. <i>Radiation Effects and Defects in Solids</i> , 2018, 173, 377-387. | 0.4 | 2 |
| 11413 | Simplified DFT methods for consistent structures and energies of large systems. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 213001. | 0.7 | 42 |
| 11414 | Probing long-range spin-spin coupling constants in 2-substituted cyclohexanones and cyclohexanethiones: the role of solvent and stereoelectronic effects. <i>Magnetic Resonance in Chemistry</i> , 2018, 56, 810-816. | 1.1 | 3 |
| 11415 | The major glucosinolate hydrolysis product in rocket (<i>Eruca sativa</i> L.), sativin, is 1,3-thiazepane-2-thione: Elucidation of structure, bioactivity, and stability compared to other rocket isothiocyanates. <i>Food Chemistry</i> , 2018, 261, 57-65. | 4.2 | 43 |
| 11416 | Optoelectronics and defect levels in hydroxyapatite by first-principles. <i>Journal of Chemical Physics</i> , 2018, 148, 154706. | 1.2 | 54 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11417 | Ab Initio Calculations of the Main Crystal Surfaces of Baryte (BaSO ₄). Crystal Growth and Design, 2018, 18, 4084-4094. | 1.4 | 10 |
| 11418 | Major differences between preferred tetracarbagallane and tetracarbalane structures. Journal of Organometallic Chemistry, 2018, 864, 88-96. | 0.8 | 1 |
| 11419 | Theoretical Determination of Energy Transfer Processes and Influence of Symmetry in Lanthanide(III) Complexes: Methodological Considerations. Inorganic Chemistry, 2018, 57, 5120-5132. | 1.9 | 27 |
| 11420 | 15-Hydroxygermacranolides as Sources of Structural Diversity: Synthesis of Sesquiterpene Lactones by Cyclization and Rearrangement Reactions. Experimental and DFT Study. Journal of Organic Chemistry, 2018, 83, 5480-5495. | 1.7 | 2 |
| 11421 | Biosynthesis and Conformational Properties of the Irregular Sesquiterpenoids Isothapsadiene and Î²-Isothapsenol. Journal of Organic Chemistry, 2018, 83, 5724-5730. | 1.7 | 2 |
| 11422 | Use of the Multilayer Fragment Molecular Orbital Method to Predict the Rank Order of Protein-Ligand Binding Affinities: A Case Study Using Tankyrase 2 Inhibitors. ACS Omega, 2018, 3, 4475-4485. | 1.6 | 14 |
| 11423 | Amide linkage in novel three-ring bent-core molecular assemblies: polar mesophases and importance of H-bonding. Liquid Crystals, 2018, 45, 1549-1566. | 0.9 | 13 |
| 11424 | Simulations of optically switchable molecular machines for particle transport. Journal of Computational Chemistry, 2018, 39, 1433-1443. | 1.5 | 4 |
| 11425 | Vibrational Sampling and Solvent Effects on the Electronic Structure of the Absorption Spectrum of 2-Nitronaphthalene. Journal of Chemical Theory and Computation, 2018, 14, 3205-3217. | 2.3 | 21 |
| 11426 | Plane-Wave Implementation and Performance of <i>À-la-Carte</i> Coulomb-Attenuated Exchange-Correlation Functionals for Predicting Optical Excitation Energies in Some Notorious Cases. Journal of Chemical Theory and Computation, 2018, 14, 3184-3195. | 2.3 | 9 |
| 11427 | Similar but Not the Same: First Kinetic and Structural Analyses of a Methanol Dehydrogenase Containing a Europium Ion in the Active Site. ChemBioChem, 2018, 19, 1147-1153. | 1.3 | 61 |
| 11428 | Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. Chemistry - A European Journal, 2018, 24, 9853-9859. | 1.7 | 28 |
| 11429 | Coumarins with an unprecedented tetracyclic skeleton and coumarin dimers from chemically engineered extracts of a marine-derived fungus. Tetrahedron, 2018, 74, 2846-2856. | 1.0 | 19 |
| 11430 | Theoretical Analysis of Optical Absorption and Emission in Mixed Noble Metal Nanoclusters. Journal of Physical Chemistry A, 2018, 122, 4058-4066. | 1.1 | 5 |
| 11431 | Triphenylstibine-substituted Fischer carbene complexes of tungsten(0): synthesis, structure, DFT and electrochemistry. New Journal of Chemistry, 2018, 42, 7301-7313. | 1.4 | 3 |
| 11432 | Nitrogen-Functionalized Hydrothermal Carbon Materials by Using Urotropine as the Nitrogen Precursor. Chemistry - A European Journal, 2018, 24, 12298-12317. | 1.7 | 16 |
| 11433 | Slow Magnetic Relaxation in a Palladium-Gadolinium Complex Induced by Electron Density Donation from the Palladium Ion. Chemistry - A European Journal, 2018, 24, 9285-9294. | 1.7 | 34 |
| 11434 | When Is Ligand p <i>K_a</i> a Good Descriptor for Catalyst Energetics? In Search of Optimal CO ₂ Hydration Catalysts. Journal of Physical Chemistry A, 2018, 122, 4579-4590. | 1.1 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11435 | Vibrational Spectroscopy of Fluoroformate, FCO_2 , Trapped in Helium Nanodroplets. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2305-2310. | 2.1 | 21 |
| 11436 | The influence of substituent field and resonance effects on the ease of N-heterocyclic carbene formation from imidazolium rings. <i>RSC Advances</i> , 2018, 8, 14833-14837. | 1.7 | 9 |
| 11437 | Electrochemical reduction of carbon dioxide with a molecular polypyridyl nickel complex. <i>Sustainable Energy and Fuels</i> , 2018, 2, 1269-1277. | 2.5 | 19 |
| 11438 | A long wavelength colourimetric chemosensor for fluoride. <i>Supramolecular Chemistry</i> , 2018, 30, 795-805. | 1.5 | 9 |
| 11439 | Hyperfine structure of Ca^{2+} molecules containing alkaline-earth-metal atoms. <i>Physical Review A</i> , 2018, 97, . | 1.0 | 14 |
| 11440 | Ab initio formation energies and time-dependent density functional theory excitation energies for nickel-nitrogen defect sites in diamond nanoparticles. <i>MRS Communications</i> , 2018, 8, 453-458. | 0.8 | 1 |
| 11441 | Synthesis, spectral characterization, DFT studies and biological activity of novel Ligand $1\text{-}(\text{cyclohexyl})\text{-}1\text{-}H\text{-}1,2,3\text{-}triazole$. <i>Overlooked Chemistry</i> , 2018, 32, e4329. | 1.7 | 14 |
| 11442 | Structural and thermochemical properties of methyl ethyl sulfide alcohols: $\text{HOCH}_2\text{SCH}_2\text{CH}_3$, $\text{CH}_3\text{SCH}_2\text{CH}_2\text{OH}$, and radicals corresponding to loss of H atom. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3836. | 0.9 | 3 |
| 11443 | Resolving the Singlet Excited State Manifold of Benzophenone by First-Principles Simulations and Ultrafast Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2570-2585. | 2.3 | 16 |
| 11444 | Tunable $\text{Rh}(\text{II})$ Light Absorbers as Excited-State Electron Donors and Acceptors Accessible with Red/Near-Infrared Irradiation. <i>Journal of the American Chemical Society</i> , 2018, 140, 5161-5170. | 6.6 | 31 |
| 11445 | Thioether- and sulfone-functionalized dibenzopentalenes as n-channel semiconductors for organic field-effect transistors. <i>Journal of Materials Chemistry C</i> , 2018, 6, 5420-5426. | 2.7 | 29 |
| 11446 | Diaryl-1,2,3-triazolylidene Platinum(II) Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 5584-5590. | 1.7 | 40 |
| 11447 | Long-Range Corrected DFT Calculations of First Hyperpolarizabilities and Excitation Energies of Metal Alkynyl Complexes. <i>ChemPhysChem</i> , 2018, 19, 1537-1546. | 1.0 | 17 |
| 11448 | Molybdenum(VI) Coordination in Tributyl Phosphate Chloride Based System. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 5661-5669. | 1.8 | 9 |
| 11449 | Dioxygenation of metal(II)-cysteinato complexes in CDO biomimetic models: Can ruthenium and osmium reach iron performances?. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25525. | 1.0 | 2 |
| 11450 | DFT calculations, crystal structure, Hirshfeld surface analyses and antibacterial studies of a new tetrachlorocuprate salt: $(\text{C}_6\text{H}_{16}\text{N}_2\text{O})[\text{CuCl}_4]$. <i>Journal of Molecular Structure</i> , 2018, 1166, 7-14. | 1.8 | 11 |
| 11451 | Resonant nonlinear microscopy reveals changes in molecular level chirality in native biological tissues. <i>Optics Communications</i> , 2018, 422, 56-63. | 1.0 | 11 |
| 11452 | Self-Interaction Error in Density Functional Theory: An Appraisal. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2353-2358. | 2.1 | 131 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 11453 | NRVS Studies of the Peroxide Shunt Intermediate in a Rieske Dioxygenase and Its Relation to the Native Fe ^{II} O ₂ Reaction. <i>Journal of the American Chemical Society</i> , 2018, 140, 5544-5559. | 6.6 | 31 |
| 11454 | Probing the structural evolution and bonding properties of Pt _n C ₂ ⁿ /O (n = 1-7) clusters by density functional calculations. <i>Chemical Physics Letters</i> , 2018, 699, 218-222. | 1.2 | 6 |
| 11455 | Unusually high stability of B ₁₂ (BO) ₁₂ achieved by boronyl ligand manipulation: Theoretical investigation. <i>Chemical Physics Letters</i> , 2018, 698, 72-76. | 1.2 | 21 |
| 11456 | Cp ₂ TiCl ₂ -catalyzed reaction of symmetrical alkynes with α,ω -dicarboxylic acid esters and Δ -tAlCl ₂ : An original pathway to 5-6 cyclic ketones and tetrasubstituted furans. <i>Tetrahedron</i> , 2018, 74, 2482-2487. | 1.0 | 4 |
| 11457 | Iron(II) and Iron(III) Spin Crossover: Toward an Optimal Density Functional. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4208-4217. | 1.1 | 79 |
| 11458 | Quantitative assessment of intermolecular interactions by atomic force microscopy imaging using copper oxide tips. <i>Nature Nanotechnology</i> , 2018, 13, 371-375. | 15.6 | 67 |
| 11459 | Benchmarking triplet-triplet annihilation photon upconversion schemes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12182-12192. | 1.3 | 19 |
| 11460 | Dissociation dynamics of 3- and 4-nitrotoluene radical cations: Coherently driven C-NO ₂ bond homolysis. <i>Journal of Chemical Physics</i> , 2018, 148, 134305. | 1.2 | 17 |
| 11461 | Vibrational tug-of-war: The pK _a dependence of the broad vibrational features of strongly hydrogen-bonded carboxylic acids. <i>Journal of Chemical Physics</i> , 2018, 148, 134309. | 1.2 | 11 |
| 11462 | Molecular excited states from the SCAN functional. <i>Molecular Physics</i> , 2018, 116, 1504-1511. | 0.8 | 8 |
| 11463 | Structural evolution dynamics in fusion of sumanenes and corannulenes: defects formation and self-healing mechanism. <i>Nano Futures</i> , 2018, 2, 025001. | 1.0 | 0 |
| 11464 | Dibenzo[a , e]pentalenophanes: Bending a Non-Alternant Hydrocarbon. <i>Chemistry - A European Journal</i> , 2018, 24, 7374-7387. | 1.7 | 36 |
| 11465 | Reverse Solvatochromism of Imine Dyes Comprised of 5-Nitrofuranyl or 5-Nitrothiophenyl as Electron Acceptor and Phenolate as Electron Donor. <i>Chemistry - A European Journal</i> , 2018, 24, 9364-9376. | 1.7 | 10 |
| 11466 | Adsorption of basic dyes onto activated carbon: Experimental and theoretical investigation of chemical reactivity of basic dyes using DFT-based descriptors. <i>Applied Surface Science</i> , 2018, 448, 662-670. | 3.1 | 124 |
| 11467 | Extracting the Americium Hydration from an Americium Cationic Mixture in Solution: A Combined X-ray Absorption Spectroscopy and Molecular Dynamics Study. <i>Inorganic Chemistry</i> , 2018, 57, 8089-8097. | 1.9 | 9 |
| 11468 | Quantum Chemical Calculation of pK _a s of Environmentally Relevant Functional Groups: Carboxylic Acids, Amines, and Thiols in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4366-4374. | 1.1 | 62 |
| 11469 | A potential method to improve the <i>in vitro</i> cytotoxicity of half-sandwich Os(^{II}) complexes against A2780 cells. <i>Dalton Transactions</i> , 2018, 47, 5714-5724. | 1.6 | 10 |
| 11470 | Effect of electric field on adsorption of formaldehyde by β -D-glucopyranose in micro-scale. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 99, 112-117. | 1.3 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11471 | Is the choice of a standard zeroth-order hamiltonian in CASPT2 ansatz optimal in calculations of excitation energies in protonated and unprotonated schiff bases of retinal?. Journal of Computational Chemistry, 2018, 39, 1470-1480. | 1.5 | 3 |
| 11472 | Recovering Intrinsic Fragmental Vibrations Using the Generalized Subsystem Vibrational Analysis. Journal of Chemical Theory and Computation, 2018, 14, 2558-2569. | 2.3 | 23 |
| 11473 | ¹³ C Kinetic Isotope Effects as a Quantitative Probe To Distinguish between Enol and Enamine Mechanisms in Aminocatalysis. Chemistry - A European Journal, 2018, 24, 8098-8102. | 1.7 | 10 |
| 11474 | Synthesis, spectroscopic characterization, DFT studies and biological activity of bis (1-(ethyl)) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Acta, 2018, 478, 222-231. | 1.2 | 15 |
| 11475 | Methyl group transfer upon gas phase decomposition of protonated methyl benzoate and similar compounds. Journal of Mass Spectrometry, 2018, 53, 379-384. | 0.7 | 3 |
| 11476 | Probing the geometric structures and electronic properties of anionic and neutral Pt3C2 clusters by density functional calculations. Chemical Physics Letters, 2018, 694, 70-74. | 1.2 | 7 |
| 11477 | Doubly hybrid density functionals that correctly describe both density and energy for atoms. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 2287-2292. | 3.3 | 36 |
| 11478 | Quantum chemical calculations of $\text{Cr}_2\text{O}_3/\text{SnO}_2$. Pramana - Journal of Physics, 2018, 90, 1. | 0.9 | 9 |
| 11479 | Carbon dioxide capture by nitrogen containing organic materials " A density functional theory investigation. Computational and Theoretical Chemistry, 2018, 1128, 1-14. | 1.1 | 6 |
| 11480 | Improving the first hyperpolarizability of anthracene through interaction with HX molecules (X F, Cl,) Tj ETQq1 1 0.784314 rgBT /Overlock 2018, 196, 353-365. | 2.0 | 4 |
| 11481 | Vibrational treatment of the formic acid double minimum case in valence coordinates. Journal of Chemical Physics, 2018, 148, 064303. | 1.2 | 22 |
| 11482 | Synthesis, molecular structure, conformation and biological activity of Ad-substituted N-aryl-tetraoxaspiroalkanes. Tetrahedron, 2018, 74, 1749-1758. | 1.0 | 22 |
| 11483 | Role of Counterions in Constant-pH Molecular Dynamics Simulations of PAMAM Dendrimers. ACS Omega, 2018, 3, 2001-2009. | 1.6 | 20 |
| 11484 | Transforming hemithioindigo from a two-way to a one-way molecular photoswitch by isolation in the gas phase. Physical Chemistry Chemical Physics, 2018, 20, 6868-6876. | 1.3 | 7 |
| 11485 | Hemisythesis, computational and molecular docking studies of novel nitrogen containing steroidal aromatase inhibitors: testolactam and testololactam. New Journal of Chemistry, 2018, 42, 4579-4589. | 1.4 | 7 |
| 11486 | Possible scenarios for SiS formation in the interstellar medium: Electronic structure calculations of the potential energy surfaces for the reactions of the SiH radical with atomic sulphur and S2. Chemical Physics Letters, 2018, 695, 87-93. | 1.2 | 33 |
| 11487 | A multidisciplinary study of 3-(β -D-glucopyranosyl)-5-substituted-1,2,4-triazole derivatives as glycogen phosphorylase inhibitors: Computation, synthesis, crystallography and kinetics reveal new potent inhibitors. European Journal of Medicinal Chemistry, 2018, 147, 266-278. | 2.6 | 22 |
| 11488 | DFT/TDDFT methods analysis of ESIPT process in a series of 7-hydroxy-1-indanone derivates and new dyad design. Journal of Saudi Chemical Society, 2018, 22, 777-785. | 2.4 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11489 | Multiple dynamics of aroylhydrazone induced by mutual effect of solvent and light - spectroscopic and computational study. <i>Journal of Molecular Liquids</i> , 2018, 255, 18-25. | 2.3 | 10 |
| 11490 | Vibrationally resolved photoelectron spectra of lower diamondoids: A time-dependent approach. <i>Journal of Chemical Physics</i> , 2018, 148, 044310. | 1.2 | 9 |
| 11491 | Ab initio periodic modelling of the vibrational spectra of molecular crystals: the case of uracil. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1. | 0.5 | 7 |
| 11492 | Gold nanoparticles as markers for fluorinated surfaces containing embedded amide groups. <i>Applied Surface Science</i> , 2018, 440, 1235-1243. | 3.1 | 0 |
| 11493 | Structure and vibrational spectroscopic study of phthalimido-functionalized N-heterocyclic palladium complexes. Correlations between structure and catalytic activity. <i>Journal of Organometallic Chemistry</i> , 2018, 869, 233-250. | 0.8 | 2 |
| 11494 | Controlling Photoconductivity in PBI Films by Supramolecular Assembly. <i>Chemistry - A European Journal</i> , 2018, 24, 4006-4010. | 1.7 | 35 |
| 11495 | Arene- π -Ligand-Free Ruthenium(II/III) Manifold for <i>meta</i> -C-H Alkylation: Remote Purine Diversification. <i>Chemistry - A European Journal</i> , 2018, 24, 3984-3988. | 1.7 | 65 |
| 11496 | Synthesis, Characterization, and Magnetic Properties of a Series of Copper(II) Chloride Complexes of Pyridyliminebenzoic Acids. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 1603-1619. | 1.0 | 8 |
| 11497 | Mechanistic insight into the ruthenium-catalyzed cycloaddition of diynes with 2,3-diphenyl-2H-azirines: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2018, 1127, 16-21. | 1.1 | 5 |
| 11498 | Li ⁺ -ligand binding energies and the effect of ligand fluorination on the binding energies. <i>Chemical Physics Letters</i> , 2018, 694, 86-92. | 1.2 | 6 |
| 11499 | Effect of torsional motion on the ¹³ C, ¹ H and ¹⁹ F NMR chemical shifts in 2,2'-difluorobiphenyl. <i>Computational and Theoretical Chemistry</i> , 2018, 1128, 42-47. | 1.1 | 0 |
| 11500 | Origin of η^2 -agostic interaction in d ⁰ transition metal alkyl complexes: Influence of ligands. <i>Journal of Organometallic Chemistry</i> , 2018, 865, 37-44. | 0.8 | 7 |
| 11501 | Novel pyridine-containing azacrownethers for the chelation of therapeutic bismuth radioisotopes: Complexation study, radiolabeling, serum stability and biodistribution. <i>Nuclear Medicine and Biology</i> , 2018, 60, 1-10. | 0.3 | 16 |
| 11502 | Experimental and Theoretical Study for Vapor Phase Aldol Condensation of Methyl Acetate and Formaldehyde over Alkali Metal Oxides Supported on SBA-15. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 2773-2786. | 1.8 | 30 |
| 11503 | Origins of Stereoselectivity in Mannich Reactions Catalyzed by Chiral Vicinal Diamines. <i>Journal of Organic Chemistry</i> , 2018, 83, 3171-3176. | 1.7 | 8 |
| 11504 | Distribution of the unpaired electron in neutral bis(phthalocyaninato) yttrium double-deckers: An experimental and theoretical combinative investigation. <i>Journal of Porphyrins and Phthalocyanines</i> , 2018, 22, 165-172. | 0.4 | 4 |
| 11505 | Polarizable Density Embedding Coupled Cluster Method. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1351-1360. | 2.3 | 20 |
| 11506 | Tuning Aromaticity of <i>para</i> -Substituted Benzene Derivatives with an External Electric Field. <i>ChemPhysChem</i> , 2018, 19, 590-595. | 1.0 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11507 | Mechanistic Unveiling of C=C Double-Bond Rotation and Origins of Regioselectivity and Product Selectivity of Pd-Catalyzed Olefinic C-H Functionalization of <i>N</i> -Methoxy Cinnamamide. <i>Journal of Organic Chemistry</i> , 2018, 83, 2067-2076. | 1.7 | 13 |
| 11508 | Ethanol Conversion to Ethylene and Acetaldehyde over Rhodium(I) Exchanged Faujasite Zeolite. A QM/MM and Microkinetic Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 2783-2795. | 1.5 | 8 |
| 11509 | Structure and adsorptive desulfurization performance of the composite material MOF-5@AC. <i>New Journal of Chemistry</i> , 2018, 42, 3840-3850. | 1.4 | 53 |
| 11510 | Comparison of Interfacial Electron Transfer Efficiency in [Fe(ctpy) ₂] ²⁺ @TiO ₂ and [Fe(cCNC) ₂] ²⁺ @TiO ₂ Assemblies: Importance of Conformational Sampling. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1821-1830. | 1.1 | 9 |
| 11511 | Electrocatalytic Reduction of CO ₂ to Formate by an Iron Schiff Base Complex. <i>Inorganic Chemistry</i> , 2018, 57, 2111-2121. | 1.9 | 97 |
| 11512 | Computational Study of the Isomerization Reactions of Borirane. <i>Journal of Organic Chemistry</i> , 2018, 83, 1804-1809. | 1.7 | 4 |
| 11513 | TDDFT Study of Charge-Transfer Raman Spectra of 4-Mercaptopyridine on Various ZnSe Nanoclusters as a Model for the SERS of 4-Mpy on Semiconductors. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4908-4927. | 1.5 | 13 |
| 11514 | <i>Ab initio</i> kinetics of the HOSO ₂ + O ₃ → SO ₃ + HO ₂ reaction. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6677-6687. | 1.3 | 15 |
| 11515 | A novel class of human 15αLOX ₁ inhibitors based on 3-hydroxycoumarin. <i>Chemical Biology and Drug Design</i> , 2018, 91, 1125-1132. | 1.5 | 11 |
| 11516 | Computational study of phenolic compounds-water clusters. <i>Structural Chemistry</i> , 2018, 29, 625-643. | 1.0 | 3 |
| 11517 | Decay of the Lowest Triplet State in Singlet-Fission Molecular Materials: A Case Study on Quinoidal Bithiophenes. <i>Journal of Physical Chemistry C</i> , 2018, 122, 3748-3755. | 1.5 | 6 |
| 11518 | Emerging investigator series: methylmercury speciation and dimethylmercury production in sulfidic solutions. <i>Environmental Sciences: Processes and Impacts</i> , 2018, 20, 584-594. | 1.7 | 17 |
| 11519 | Theoretical Prediction of Activation Free Energies of Various Hydride Self-Exchange Reactions in Acetonitrile at 298 K. <i>ACS Omega</i> , 2018, 3, 872-885. | 1.6 | 16 |
| 11520 | A Comparative IRMPD and DFT Study of Fe ³⁺ and UO ₂ ²⁺ Complexation with <i>N</i> -Methylacetohydroxamic Acid. <i>Inorganic Chemistry</i> , 2018, 57, 1125-1135. | 1.9 | 13 |
| 11521 | The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. <i>Photochemical and Photobiological Sciences</i> , 2018, 17, 323-331. | 1.6 | 10 |
| 11522 | Efficient evaluation of atom tunneling combined with electronic structure calculations. <i>Journal of Chemical Physics</i> , 2018, 148, 102334. | 1.2 | 23 |
| 11523 | Synthesis, photophysical, structural and electronic properties of novel regioisomerically pure 1,7-disubstituted perylene-3,4,9,10-tetracarboxylic monoimide dibutylester derivatives. <i>Journal of Molecular Structure</i> , 2018, 1158, 145-155. | 1.8 | 7 |
| 11524 | What Gives an Insulin Hexamer Its Unique Shape and Stability? Role of Ten Confined Water Molecules. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1631-1637. | 1.2 | 39 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11525 | Changing molecular conjugation with a phenazine acceptor for improvement of small molecule-based organic electronic memory performance. <i>RSC Advances</i> , 2018, 8, 805-811. | 1.7 | 11 |
| 11526 | Competing Pathways in the Photochemistry of Ru(H) ₂ (CO)(PPh ₃) ₃ . <i>Organometallics</i> , 2018, 37, 855-868. | 1.1 | 8 |
| 11527 | Design of highly selective ethanol dehydration nanocatalysts for ethylene production. <i>Nanoscale</i> , 2018, 10, 4004-4009. | 2.8 | 10 |
| 11528 | Introducing DDEC6 atomic population analysis: part 4. Efficient parallel computation of net atomic charges, atomic spin moments, bond orders, and more. <i>RSC Advances</i> , 2018, 8, 2678-2707. | 1.7 | 129 |
| 11529 | A numerical and experimental study of the decomposition pathways of guanidinium nitrate. <i>Journal of Thermal Analysis and Calorimetry</i> , 2018, 131, 427-441. | 2.0 | 7 |
| 11530 | Electron Pair Repulsion Responsible for the Peculiar Edge Effects and Surface Chemistry of Black Phosphorus. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 947-953. | 2.1 | 15 |
| 11531 | An electrically conducting crystal composed of an octahedrally ligated porphyrin complex with high-spin iron (iii). <i>Dalton Transactions</i> , 2018, 47, 4070-4075. | 1.6 | 3 |
| 11532 | Three-Component Activation/Alkynylation/Cyclocondensation (AACC) Synthesis of Enhanced Emission Solvatochromic 3-Ethynylquinoxalines. <i>Chemistry - A European Journal</i> , 2018, 24, 8114-8125. | 1.7 | 22 |
| 11533 | Accelerating Chemical Discovery with Machine Learning: Simulated Evolution of Spin Crossover Complexes with an Artificial Neural Network. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1064-1071. | 2.1 | 145 |
| 11534 | A computational study of the interplay of steric and electronic effects in the stabilization of 1,3-(diamino)oxyallyls. <i>Journal of Molecular Structure</i> , 2018, 1172, 3-7. | 1.8 | 6 |
| 11535 | Thiocarbonyl-bound metallonitrosyl complexes with visible-light induced DNA cleavage and promising vasodilation activity. <i>Journal of Inorganic Biochemistry</i> , 2018, 182, 83-91. | 1.5 | 19 |
| 11536 | Singlet-triplet splittings from the virial theorem and single-particle excitation energies. <i>Journal of Chemical Physics</i> , 2018, 148, 044112. | 1.2 | 19 |
| 11537 | Effects of Ta ₂ O ₅ Surface Modification by NH ₃ on the Electronic Structure of a Ru-Complex/N-Ta ₂ O ₅ Hybrid Photocatalyst for Selective CO ₂ Reduction. <i>Journal of Physical Chemistry C</i> , 2018, 122, 1921-1929. | 1.5 | 12 |
| 11538 | A Copper(II) Nitrite That Exhibits Change of Nitrite Binding Mode and Formation of Copper(II) Nitrosyl Prior to Nitric Oxide Evolution. <i>Inorganic Chemistry</i> , 2018, 57, 1550-1561. | 1.9 | 19 |
| 11539 | Bright green-to-yellow emitting Cu(II) complexes based on bis(2-pyridyl)phosphine oxides: synthesis, structure and effective thermally activated-delayed fluorescence. <i>Dalton Transactions</i> , 2018, 47, 2701-2710. | 1.6 | 33 |
| 11540 | Probing Cyclic π -Electron Delocalization in an Imidazol π -ylidene and a Corresponding Imidazolium Salt. <i>Chemistry - A European Journal</i> , 2018, 24, 4973-4981. | 1.7 | 8 |
| 11541 | Controlling the crystallinity and crystalline orientation of α -shuttlecock-naphthalocyanine films for near-infrared optoelectronic applications. <i>Journal of Materials Chemistry C</i> , 2018, 6, 1959-1970. | 2.7 | 8 |
| 11542 | Iron(II)-Catalyzed Hydrogenation of Acetophenone with a Chiral, Pyridine-Based PNP Pincer Ligand: Support for an Outer-Sphere Mechanism. <i>Organometallics</i> , 2018, 37, 396-405. | 1.1 | 50 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11543 | Synthesis and magneto-structural studies on a new family of carbonato bridged 3d ⁴ complexes featuring a [Coll ₃ LnIII ₃ (CO ₃) ₃] (Ln = La, Gd, Tb, Dy and Ho) core: slow magnetic relaxation displayed by the cobalt(II)–dysprosium(III) analogue. <i>Dalton Transactions</i> , 2018, 47, 3425-3439. | 1.6 | 18 |
| 11544 | Direct observation of 4-nitrophenyl disulfide produced from p-nitrothiophenol in air by Raman spectroscopy. <i>Journal of Raman Spectroscopy</i> , 2018, 49, 520-525. | 1.2 | 4 |
| 11545 | DFT study on λ -regioselectivity of photo-organocatalytic functionalization of aldehydes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 355, 9-15. | 2.0 | 0 |
| 11546 | Stabilization of Ni ²⁺ dimers in hexacyano Mo ₆ cluster-based Prussian blue derivatives: experimental and theoretical investigations of magnetic properties. <i>Dalton Transactions</i> , 2018, 47, 1122-1130. | 1.6 | 5 |
| 11547 | Stepwise synthesis of the heterotrimetallic chains [MRu ₂ (dpa) ₄ X ₂] ^{0/1+} using group 7 to group 12 transition metal ions and [Ru ₂ (dpa) ₄ Cl]. <i>Dalton Transactions</i> , 2018, 47, 1422-1434. | 1.6 | 21 |
| 11548 | ETS-NOCV decomposition of the reaction force for double-proton transfer in formamide-derived systems. <i>Journal of Molecular Modeling</i> , 2018, 24, 27. | 0.8 | 7 |
| 11549 | Structural, electronic, and reactivity parameters of some triorganotin(IV) carboxylates: a DFT analysis. <i>Structural Chemistry</i> , 2018, 29, 753-763. | 1.0 | 9 |
| 11550 | Citronellal assumes a folded conformation in solution due to dispersion interactions: A joint NMR-DFT analysis. <i>Journal of Molecular Structure</i> , 2018, 1157, 401-407. | 1.8 | 5 |
| 11551 | Theoretical study on the reaction mechanism of Pd(OAc) ₂ -catalyzed trifluoroethylation: Role of additive CF ₃ COOH. <i>Tetrahedron Letters</i> , 2018, 59, 462-468. | 0.7 | 6 |
| 11552 | Evaluations of the accuracies of DMol3 density functionals for calculations of experimental binding enthalpies of N ₂ , CO, H ₂ , C ₂ H ₂ at catalytic metal sites. <i>Molecular Simulation</i> , 2018, 44, 568-581. | 0.9 | 38 |
| 11553 | 1,2,4-triazole derivatives with morpholine; DFT study and antileishmanial activity. <i>Canadian Journal of Physics</i> , 2018, 96, 719-723. | 0.4 | 5 |
| 11554 | Exploring the relevance of thiophene rings as bridge unit in acceptor–bridge–donor dyes on self-assembly and performance in DSSCs. <i>Journal of Computational Chemistry</i> , 2018, 39, 685-698. | 1.5 | 10 |
| 11555 | A computational study of PAMAM dendrimer interaction with trans isomer of picoplatin anticancer drug. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 80, 1-6. | 1.3 | 11 |
| 11556 | Nitrido complex of high-valent Ru(VI) -catalyzed reduction of imines and alkynes with hydrosilanes: A theoretical study of the reaction mechanism. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 2-11. | 0.8 | 6 |
| 11557 | Quantum chemical predictions of aqueous pK values for OH groups of some λ -hydroxycarboxylic acids based on ab initio and DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2018, 1125, 29-38. | 1.1 | 19 |
| 11558 | Synthesis of hexavalent molybdenum formo- and aceto-hydroxamates and deferoxamine via liquid-liquid metal partitioning. <i>Inorganica Chimica Acta</i> , 2018, 473, 102-111. | 1.2 | 6 |
| 11559 | Mechanistic insights into tandem amine-borane dehydrogenation and alkene hydrogenation catalyzed by [Pd(NHC)(PCy ₃)]. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 2043-2049. | 3.8 | 3 |
| 11560 | Investigation of Strain-Promoted Azide–Alkyne Cycloadditions in Aqueous Solutions by Capillary Electrophoresis. <i>Journal of Organic Chemistry</i> , 2018, 83, 604-613. | 1.7 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11561 | Superposed Redox Chemistry of Fused Carbon Rings in Cyclooctatetraene-Based Organic Molecules for High-Voltage and High-Capacity Cathodes. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 2496-2503. | 4.0 | 12 |
| 11562 | TGA, Hirshfeld, Raman spectroscopy and computational studies of diethylammonium hexachloroplumbate [(C ₂ H ₅) ₂ NH ₂] ₂ PbCl ₆ . <i>Journal of Molecular Structure</i> , 2018, 1157, 621-630. | 1.8 | 5 |
| 11563 | Wannier Koopmans Method Calculations of 2D Material Band Gaps. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 281-285. | 2.1 | 12 |
| 11564 | New electron delocalization tools to describe the aromaticity in porphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2787-2796. | 1.3 | 86 |
| 11565 | <sc>SERS</sc> spectrum of imazalil. Experimental and quantumâ€chemical vibrational analysis. <i>Journal of Raman Spectroscopy</i> , 2018, 49, 638-650. | 1.2 | 4 |
| 11566 | Structural, optical, and thermal properties of MAX-phase Cr ₂ AlB ₂ . <i>Frontiers of Physics</i> , 2018, 13, 1. | 2.4 | 10 |
| 11567 | Computational investigation of the structure and antioxidant activity of some pyrazole and pyrazolone derivatives. <i>Journal of Saudi Chemical Society</i> , 2018, 22, 705-714. | 2.4 | 31 |
| 11568 | Dissecting the Gold(I)-Catalyzed Carboaminations of <i>N</i>-Allyl Tetrahydro-Î ² -carbolines to Allenes. <i>Journal of Organic Chemistry</i> , 2018, 83, 898-912. | 1.7 | 9 |
| 11569 | Understanding the structure and reactivity of the Câ€S linkage in biologically active 5-arythio-5<i>H</i>-chromenopyridines. <i>New Journal of Chemistry</i> , 2018, 42, 1151-1158. | 1.4 | 12 |
| 11570 | Synthesis and Unusual NMRâ€Spectroscopic Behavior of a Strained Bicyclic Ammonium Salt. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 1204-1207. | 1.2 | 2 |
| 11571 | How reliable are Minnesota density functionals for modeling phosphorusâ€hydrogen NMR spinâ€spin coupling constants?. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1. | 0.5 | 3 |
| 11572 | Theoretical design on a new double functional device of 2,2â€bipyridineâ€embedded <sc><i>N</i></sc>-â€(9â€pyrenyl methyl)azaâ€15â€crownâ€5. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, 0.9 e3792. | | 2 |
| 11573 | Rational Density Functional Selection Using Game Theory. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 61-67. | 2.5 | 20 |
| 11574 | Atom-Centered Potentials with Dispersion-Corrected Minimal-Basis-Set Hartreeâ€Fock: An Efficient and Accurate Computational Approach for Large Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 726-738. | 2.3 | 18 |
| 11575 | New Ligand Design Provides Delocalization and Promotes Strong Absorption throughout the Visible Region in a Ru(II) Complex. <i>Journal of the American Chemical Society</i> , 2018, 140, 229-234. | 6.6 | 39 |
| 11576 | Novel high temperature polymeric encapsulation material for extreme environment electronics packaging. <i>Materials and Design</i> , 2018, 141, 202-209. | 3.3 | 34 |
| 11577 | Mechanism and <i>cis</i>/<i>trans</i> Selectivity of Vinylogous Nazarov-type [6Î] Photocyclizations. <i>Journal of Organic Chemistry</i> , 2018, 83, 964-972. | 1.7 | 16 |
| 11578 | Oxidative Coupling Mechanisms: Current State of Understanding. <i>ACS Catalysis</i> , 2018, 8, 1161-1172. | 5.5 | 83 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 11579 | Characterisation of the electronic structure of galvinoxyl free radical by variable energy UPS, XPS and NEXAFS spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2480-2491. | 1.3 | 11 |
| 11580 | One-step coelectrodeposition-assisted layer-by-layer assembly of gold nanoparticles and reduced graphene oxide and its self-healing three-dimensional nanohybrid for an ultrasensitive DNA sensor. <i>Nanoscale</i> , 2018, 10, 1196-1206. | 2.8 | 48 |
| 11581 | Ƴf-Holes and Ƴf-lumps direct the Lewis basic and acidic interactions of noble metal nanoparticles: introducing regium bonds. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2676-2692. | 1.3 | 99 |
| 11582 | Luminescent Dinuclear Copper(I) Complexes as Potential Thermally Activated Delayed Fluorescence (TADF) Emitters: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1413-1421. | 1.1 | 34 |
| 11583 | Covalently bonded 2D/2D O-g-C ₃ N ₄ /TiO ₂ heterojunction for enhanced visible-light photocatalytic hydrogen evolution. <i>Applied Catalysis B: Environmental</i> , 2018, 237, 1130-1138. | 10.8 | 129 |
| 11584 | Water-Assisted Hole Trapping at the Highly Curved Surface of Nano-TiO ₂ Photocatalyst. <i>Journal of the American Chemical Society</i> , 2018, 140, 1415-1422. | 6.6 | 95 |
| 11585 | Studies on hydroquinone based maleate bolaamphiphile organogels and their drug formulations. <i>Soft Materials</i> , 2018, 16, 108-116. | 0.8 | 7 |
| 11586 | Functionalization of fluorodinitroethylamino derivatives based on azole: a new family of insensitive energetic materials. <i>New Journal of Chemistry</i> , 2018, 42, 2994-3000. | 1.4 | 10 |
| 11587 | Combined spectroscopic, molecular docking and quantum mechanics study of Ƴ ² -casein and p-coumaric acid interactions following thermal treatment. <i>Food Chemistry</i> , 2018, 252, 163-170. | 4.2 | 60 |
| 11588 | Theoretical Insights into Imidazolidine Oxidation of Imidacloprid by Cytochrome P450 3A4. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 80, 173-181. | 1.3 | 8 |
| 11589 | Theoretical studies on copper-catalyzed arylation of nitrogen heterocycles from benzenediazonium acetate under ligand-free conditions. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 50-57. | 0.8 | 10 |
| 11590 | Density Functional Theory Study on the Demethylation Reaction between Methylamine, Dimethylamine, Trimethylamine, and Tamoxifen Catalyzed by a Fe(IV) Ƴ-oxo Porphyrin Complex. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1658-1671. | 1.1 | 8 |
| 11591 | Theoretical insight into the mechanisms of palladium-catalyzed intramolecular insertion of alkenes into the carbon-nitrogen bond of Ƴ ² -lactam. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 37-43. | 0.8 | 3 |
| 11592 | Static polarizabilities and optical absorption spectra of boron clusters (n = 20, 38 and 40) using first principles. <i>Computational and Theoretical Chemistry</i> , 2018, 1125, 54-62. | 1.1 | 8 |
| 11593 | The High Performance of Choline Arginate for Biomass Pretreatment Is Due to Remarkably Strong Hydrogen Bonding by the Anion. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 4115-4121. | 3.2 | 18 |
| 11594 | Unexpected cleavage of upper rim-bridged calix[4]arenes leading to linear oligophenolic derivatives. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 838-843. | 1.5 | 6 |
| 11595 | Ultrasensitive and specific fluorescence detection of a cancer biomarker via nanomolar binding to a guanidinium-modified calixarene. <i>Chemical Science</i> , 2018, 9, 2087-2091. | 3.7 | 113 |
| 11596 | Relativistic effects on inversion barriers of pyramidal group 15 hydrides. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25585. | 1.0 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 11597 | Effect of chain length on the interactions of sodium N-alkyl prolinates with bovine serum albumin: a spectroscopic investigation and molecular docking simulations. <i>Colloid and Polymer Science</i> , 2018, 296, 367-378. | 1.0 | 6 |
| 11598 | A theoretical study on La-activated bicyclo-oligomerization of acetylene to form naphthalene in gas phase using density functional theory (DFT). <i>Structural Chemistry</i> , 2018, 29, 171-178. | 1.0 | 3 |
| 11599 | Zinc and copper complexes of stilbene iminopyridine ligands with η^2 -Olefin binding mode. <i>Journal of Organometallic Chemistry</i> , 2018, 858, 14-22. | 0.8 | 4 |
| 11600 | A selective "turn-on" fluorescent chemosensor for detection of Al ³⁺ in aqueous medium: Experimental and theoretical studies. <i>Sensors and Actuators B: Chemical</i> , 2018, 260, 888-899. | 4.0 | 93 |
| 11601 | Structural Evolution of B ₂ Si _n ($n = 3-12$) Clusters: Size-Selected Anion Photoelectron Spectroscopy and Theoretical Calculations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 2391-2401. | 1.5 | 31 |
| 11602 | Homogeneously Catalyzed Electroreduction of Carbon Dioxide—Methods, Mechanisms, and Catalysts. <i>Chemical Reviews</i> , 2018, 118, 4631-4701. | 23.0 | 858 |
| 11603 | Synthesis and application of a water-soluble phosphorescent iridium complex as turn-on sensing material for human serum albumin. <i>Dalton Transactions</i> , 2018, 47, 2330-2336. | 1.6 | 16 |
| 11604 | Serenity: A subsystem quantum chemistry program. <i>Journal of Computational Chemistry</i> , 2018, 39, 788-798. | 1.5 | 57 |
| 11605 | Ab initio calculation of nonlinear optical properties for chiral carbon nanotubes. Second harmonic generation and dc-Pockels effect. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1. | 0.5 | 4 |
| 11606 | How to tame a palladium terminal imido. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 26-36. | 0.8 | 14 |
| 11607 | Synthesis, characterization, single crystal X-ray and DFT analysis of disubstituted phosphorodithioates. <i>Journal of Molecular Structure</i> , 2018, 1157, 708-715. | 1.8 | 8 |
| 11608 | Absolute and relative facial selectivities in organocatalytic asymmetric chlorocyclization reactions. <i>Chemical Science</i> , 2018, 9, 2898-2908. | 3.7 | 22 |
| 11609 | Solvent effect on the degree of (a)synchronicity in polar Diels-Alder reactions from the perspective of the reaction force constant analysis. <i>Journal of Molecular Modeling</i> , 2018, 24, 33. | 0.8 | 6 |
| 11610 | Mg/Ga mixed-oxide catalysts for phenol methylation: Outstanding performance in 2,4,6-trimethylphenol synthesis with co-feeding of water. <i>Applied Catalysis A: General</i> , 2018, 552, 86-97. | 2.2 | 22 |
| 11611 | Challenges in XUV Photochemistry Simulations: A Case Study on Ultrafast Fragmentation Dynamics of the Benzene Radical Cation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1004-1010. | 1.1 | 10 |
| 11612 | Ligand substitution and conformational effects on the ultrafast luminescent decay of [Re(CO) ₃ (phen)(L)] ⁺ (L = imidazole, pyridine): non-adiabatic quantum dynamics. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1134-1141. | 1.3 | 22 |
| 11613 | Benchmark-Quality Semiexperimental Structural Parameters of van der Waals Complexes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1077-1087. | 1.1 | 16 |
| 11614 | Kinetics of the Methanol Reaction with OH at Interstellar, Atmospheric, and Combustion Temperatures. <i>Journal of the American Chemical Society</i> , 2018, 140, 2906-2918. | 6.6 | 100 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11615 | BAR-based optimum adaptive sampling regime for variance minimization in alchemical transformation: the nonequilibrium stratification. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2009-2021. | 1.3 | 31 |
| 11616 | Azetidinium-based Hypergolic Ionic Liquids with High Strain Energy. <i>ChemistrySelect</i> , 2018, 3, 284-288. | 0.7 | 7 |
| 11617 | Where Does the Density Localize in the Solid State? Divergent Behavior for Hybrids and DFT+U. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 670-683. | 2.3 | 57 |
| 11618 | Theoretical and experimental study of triphenylphosphonium Schiff base of 5-hydroxy-3-methyl-1-phenyl-4-formylpyrazole. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2018, 193, 375-381. | 0.8 | 3 |
| 11619 | Synthesis and Structural Features of a Lithium Borate Derived from 2,2-Dipropylglycolic Acid. <i>Bulletin of the Chemical Society of Japan</i> , 2018, 91, 12-18. | 2.0 | 1 |
| 11620 | Benchmark CCSD(T) and DFT study of binding energies in Be ₇ ⁺ : in search of reliable DFT functional for beryllium clusters. <i>Molecular Physics</i> , 2018, 116, 1259-1274. | 0.8 | 9 |
| 11621 | Structuring Conjugated Polymers and Polyelectrolytes Through Self-Assembly. <i>Materials and Energy</i> , 2018, , 67-114. | 2.5 | 0 |
| 11622 | Theoretical investigations on copper catalyzed C N cross-coupling reaction between aryl chlorides and amines. <i>Computational and Theoretical Chemistry</i> , 2018, 1134, 1-7. | 1.1 | 8 |
| 11623 | Theoretical Investigation on Direct Vinylogous Aldol Reaction of Isatin Catalyzed by Chiral- N , N' -dioxide Sc(III) Complex. <i>Molecular Catalysis</i> , 2018, 453, 22-30. | 1.0 | 1 |
| 11624 | Enhancing the Kinetic Stability and Lifetime of Organic Light-Emitting Diodes based on Bipolar Hosts by using Spiroconjugation. <i>ChemPhysChem</i> , 2018, 19, 1711-1715. | 1.0 | 3 |
| 11625 | Superbase-catalyzed domino 3 <i>H</i> -pyrroles synthesis from ketoximes and acetylene: DFT study vs experiment. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3829. | 0.9 | 7 |
| 11626 | Diversity-oriented four-component synthesis of solid state luminescent difluoro oxazaborinines. <i>Dyes and Pigments</i> , 2018, 157, 198-217. | 2.0 | 10 |
| 11627 | Desorption of Benzene, 1,3,5-Trifluorobenzene, and Hexafluorobenzene from a Graphene Surface: The Effect of Lateral Interactions on the Desorption Kinetics. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2632-2638. | 2.1 | 4 |
| 11628 | Nascent energy distribution of the Criegee intermediate CH ₂ OO from direct dynamics calculations of primary ozonide dissociation. <i>Journal of Chemical Physics</i> , 2018, 148, 174306. | 1.2 | 36 |
| 11629 | Tetrasubstituted bisadamantylidenes Highly twisted alkenes. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3840. | 0.9 | 3 |
| 11630 | Quinine-Promoted, Enantioselective Boron-Tethered Diels-Alder Reaction by Anomeric Control of Transition-State Conformation. <i>Journal of Organic Chemistry</i> , 2018, 83, 5756-5765. | 1.7 | 15 |
| 11631 | Preferential Solvation Unveiled by Anomalous Conformational Equilibration of Porphyrin Dimers: Nucleation Growth of Solvent-Solvent Segregation. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5251-5259. | 1.2 | 15 |
| 11632 | A rare example of a compact heteroleptic cyclometalated iridium(III) complex demonstrating well-separated dual emission. <i>Dalton Transactions</i> , 2018, 47, 7578-7586. | 1.6 | 22 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11633 | Size-scaling behaviour of the electronic polarizability of one-dimensional interacting systems. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 175603. | 0.7 | 3 |
| 11634 | First-principle calculations of electronic structures and polar properties of (I ^ε ,I ^μ)-Ga ₂ O ₃ . <i>Applied Physics Express</i> , 2018, 11, 061101. | 1.1 | 53 |
| 11635 | Oxidation of 7-ethyl-2,3,5,6,8-pentahydroxy-1,4-naphthoquinone (echinochrome A) by atmospheric oxygen 1. Structure of dehydroechinochrome. <i>Russian Chemical Bulletin</i> , 2018, 67, 282-290. | 0.4 | 8 |
| 11636 | Effects of Halogen and Hydrogen Bonding on the Electronics of a Conjugated Rotor. <i>Journal of Organic Chemistry</i> , 2018, 83, 6142-6150. | 1.7 | 5 |
| 11637 | Substituent Effect in the First Excited Singlet State of Monosubstituted Benzenes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4609-4621. | 1.1 | 21 |
| 11638 | Structural characterization of the P1+ intermediate state of the P-cluster of nitrogenase. <i>Journal of Biological Chemistry</i> , 2018, 293, 9629-9635. | 1.6 | 44 |
| 11639 | Total Synthesis of Natural Hyacinthacine C ₅ and Six Related Hyacinthacine C ₅ Epimers. <i>Journal of Organic Chemistry</i> , 2018, 83, 5558-5576. | 1.7 | 25 |
| 11640 | O-Regioselective Synthesis with the Silver Salt Method. <i>ACS Omega</i> , 2018, 3, 4557-4572. | 1.6 | 7 |
| 11641 | Reaction Mechanism and Kinetics for Ammonia Synthesis on the Fe(111) Surface. <i>Journal of the American Chemical Society</i> , 2018, 140, 6288-6297. | 6.6 | 126 |
| 11642 | Structural analysis of benzothienobenzothiophene-based soluble organic semiconducting crystals grown by liquid crystal solvent. <i>Journal of Crystal Growth</i> , 2018, 492, 98-104. | 0.7 | 5 |
| 11643 | Considerations of nano-QSAR/QSPR models for nanopesticide risk assessment within the European legislative framework. <i>Science of the Total Environment</i> , 2018, 634, 1530-1539. | 3.9 | 74 |
| 11644 | Iron versus Ruthenium: Clarifying the Electronic Differences between Prototypical Mixed-Valence Organometallic Butadiynyl Bridged Molecular Wires. <i>Organometallics</i> , 2018, 37, 1432-1445. | 1.1 | 44 |
| 11645 | A combined theoretical and experimental study of the ultrafast photophysics of Rhodamine B. <i>Molecular Physics</i> , 2018, 116, 2162-2171. | 0.8 | 7 |
| 11646 | Strong Preference of the Redox-Neutral Mechanism over the Redox Mechanism for the Ti ^{IV} Catalysis Involved in the Carboamination of Alkyne with Alkene and Diazene. <i>Chemistry - A European Journal</i> , 2018, 24, 7010-7025. | 1.7 | 12 |
| 11647 | Arynes and Cyclic Alkynes as Synthetic Building Blocks for Stereodefined Quaternary Centers. <i>Journal of the American Chemical Society</i> , 2018, 140, 7605-7610. | 6.6 | 40 |
| 11648 | Rotational Isomers, Intramolecular Hydrogen Bond, and IR Spectra of o-Vinylphenol Homologs. <i>Journal of Applied Spectroscopy</i> , 2018, 85, 9-20. | 0.3 | 1 |
| 11649 | Theoretical studies on bridged frustrated Lewis pair (FLP) mediated H ₂ activation and CO ₂ hydrogenation. <i>Organic Chemistry Frontiers</i> , 2018, 5, 1905-1915. | 2.3 | 26 |
| 11650 | Simplified calculation approaches designed to reproduce the geometry of hydrogen bonds in molecular complexes in aprotic solvents. <i>Journal of Chemical Physics</i> , 2018, 148, 124313. | 1.2 | 21 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11651 | Alchemical and structural distribution based representation for universal quantum machine learning. <i>Journal of Chemical Physics</i> , 2018, 148, 241717. | 1.2 | 272 |
| 11652 | Interstate vibronic coupling constants between electronic excited states for complex molecules. <i>Journal of Chemical Physics</i> , 2018, 148, 124119. | 1.2 | 33 |
| 11653 | Calculation of Ligand Dissociation Energies in Large Transition-Metal Complexes. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2456-2468. | 2.3 | 62 |
| 11654 | Absorption Refrigeration Cycles with Ammonia-Ionic Liquid Working Pairs Studied by Molecular Simulation. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 5442-5452. | 1.8 | 39 |
| 11655 | Synthesis and nonlinear optical properties of novel conjugated small molecules based on indole donor. <i>Journal of Molecular Structure</i> , 2018, 1165, 223-227. | 1.8 | 19 |
| 11656 | Ammonia Activation by Ce Atom: Matrix-Isolation FTIR and Theoretical Studies. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3541-3546. | 1.1 | 4 |
| 11657 | Self-assembly study of nanometric spheres from polyoxometalate-phenylalanine hybrids, an experimental and theoretical approach. <i>Dalton Transactions</i> , 2018, 47, 6304-6313. | 1.6 | 30 |
| 11658 | Investigating the Interaction of Silicon Dioxide Nanoparticles with Human Hemoglobin and Lymphocyte Cells by Biophysical, Computational, and Cellular Studies. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4278-4288. | 1.2 | 36 |
| 11659 | Predicting an unconventional facile route to metallaanthracenes. <i>Dalton Transactions</i> , 2018, 47, 5575-5581. | 1.6 | 8 |
| 11660 | Generalized Density-Functional Tight-Binding Repulsive Potentials from Unsupervised Machine Learning. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2341-2352. | 2.3 | 44 |
| 11661 | Arylketone π -Conjugation Controls Enantioselectivity in Asymmetric Alkynylations Catalyzed by Centrochiral Ruthenium Complexes. <i>Journal of the American Chemical Society</i> , 2018, 140, 5146-5152. | 6.6 | 26 |
| 11662 | Reversible modulation of the redox characteristics of acid-sensitive molybdenum and tungsten scorpionate complexes. <i>Dalton Transactions</i> , 2018, 47, 6323-6332. | 1.6 | 10 |
| 11663 | Influences of donor/acceptor ratio on the optical and electrical properties of the D/A alternating model oligomers: A density functional theory study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 199, 260-270. | 2.0 | 2 |
| 11664 | Raman spectroscopic discrimination of estrogens. <i>Vibrational Spectroscopy</i> , 2018, 96, 93-100. | 1.2 | 10 |
| 11665 | Computational Study of the Structure and Degradation Products of Alloxidim Herbicide. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3909-3918. | 1.1 | 7 |
| 11666 | Spin-Switching Transmetalation at Ni Diimine Catalysts. <i>ACS Catalysis</i> , 2018, 8, 3655-3666. | 5.5 | 20 |
| 11667 | A theoretical mechanistic study on electrical conductivity enhancement of DMSO treated PEDOT:PSS. <i>Journal of Materials Chemistry C</i> , 2018, 6, 5122-5131. | 2.7 | 100 |
| 11668 | Theoretical insights on the C-C bond reductive elimination from Co(III) center. <i>Computational and Theoretical Chemistry</i> , 2018, 1130, 140-147. | 1.1 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11669 | Reductive Defluorination of Branched Per- and Polyfluoroalkyl Substances with Cobalt Complex Catalysts. <i>Environmental Science and Technology Letters</i> , 2018, 5, 289-294. | 3.9 | 65 |
| 11670 | Spin-orbital model of stoichiometric LaMnO_3 with tetragonal distortions. <i>Physical Review B</i> , 2018, 97, . | 1.1 | 2 |
| 11671 | Noncovalent Interactions Descriptor Based on the Source Function of Individual Localized Molecular Orbitals in Whole Space. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3850-3857. | 1.1 | 2 |
| 11672 | Density functional theory modeling of chromate adsorption onto ferrihydrite nanoparticles. <i>Geochemical Transactions</i> , 2018, 19, 8. | 1.8 | 26 |
| 11673 | Identifying intermediates in the reductive intramolecular cyclisation of allyl 2-bromobenzyl ether by an improved electron paramagnetic resonance spectroelectrochemical electrode design combined with density functional theory calculations. <i>Electrochimica Acta</i> , 2018, 271, 10-18. | 2.6 | 10 |
| 11674 | Extension of the GROMOS 56a6 CARBO/CARBO_R Force Field for Charged, Protonated, and Esterified Uronates. <i>Journal of Physical Chemistry B</i> , 2018, 122, 3696-3710. | 1.2 | 17 |
| 11675 | Computational design of boron doped lithium (BLi _n) cluster-based catalyst for N ₂ fixation. <i>Computational and Theoretical Chemistry</i> , 2018, 1130, 107-112. | 1.1 | 3 |
| 11676 | Accurate prediction of bond dissociation energies of large n-alkanes using ONIOM-CCSD(T)/CBS methods. <i>Chemical Physics Letters</i> , 2018, 699, 139-145. | 1.2 | 10 |
| 11677 | A Well-Tempered Hybrid Method for Solving Challenging Time-Dependent Density Functional Theory (TDDFT) Systems. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2034-2041. | 2.3 | 15 |
| 11678 | Understanding titanium-catalysed radical reactions: a DFT study unravels the complex kinetics of ketone nitrile couplings. <i>Dalton Transactions</i> , 2018, 47, 5072-5082. | 1.6 | 18 |
| 11679 | Sulfonamide derivatives as Mycobacterium tuberculosis inhibitors: in silico approach. <i>In Silico Pharmacology</i> , 2018, 6, 4. | 1.8 | 13 |
| 11680 | Magneto-Structural Properties and Theoretical Studies of a Family of Simple Heterodinuclear Phenoxide/Alkoxide Bridged Mn ^{III} Ln ^{III} Complexes: On the Nature of the Magnetic Exchange and Magnetic Anisotropy. <i>Inorganic Chemistry</i> , 2018, 57, 3683-3698. | 1.9 | 37 |
| 11681 | An accurate first-principles treatment of doping-dependent electronic structure of high-temperature cuprate superconductors. <i>Communications Physics</i> , 2018, 1, . | 2.0 | 94 |
| 11682 | Non-covalent interaction in benzene and substituted benzene: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2018, 1130, 134-139. | 1.1 | 29 |
| 11683 | Spin-Orbit Splittings and Low-Lying Electronic States of AuSi and AuGe: Anion Photoelectron Spectroscopy and <i>ab Initio</i> Calculations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3374-3382. | 1.1 | 13 |
| 11684 | Probing the antioxidant potential of phloretin and phlorizin through a computational investigation. <i>Journal of Molecular Modeling</i> , 2018, 24, 101. | 0.8 | 40 |
| 11685 | Synthesis of t-butyl 2-(4-hydroxy-3-methoxybenzylidene)hydrazine carboxylate: Experimental and theoretical investigations of its properties. <i>Journal of Molecular Structure</i> , 2018, 1164, 516-524. | 1.8 | 22 |
| 11686 | Modeling L _{2,3} -Edge X-ray Absorption Spectroscopy with Real-Time Exact Two-Component Relativistic Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1998-2006. | 2.3 | 44 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11687 | Methylmercury interferes with glucocorticoid receptor: Potential role in the mediation of developmental neurotoxicity. <i>Toxicology and Applied Pharmacology</i> , 2018, 354, 94-100. | 1.3 | 17 |
| 11688 | Bromine atom promoted C-H bond activation in terminal alkynes at room temperature on Ag(111). <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 11081-11088. | 1.3 | 35 |
| 11689 | Cooperativity in spin crossover materials as ligand's responsibility – investigations of the Fe(<i>ii</i>) – 1,3-bis((1 <i>H</i> -tetrazol-1-yl)methyl)bicyclo[1.1.1]pentane system. <i>Dalton Transactions</i> , 2018, 47, 5553-5557. | 1.6 | 5 |
| 11690 | Energy transfer or electron transfer? – DFT study on the mechanism of [2+2] cycloadditions induced by visible light photocatalysts. <i>Tetrahedron Letters</i> , 2018, 59, 1651-1660. | 0.7 | 6 |
| 11691 | Dopant-Dependent SFG Response of Rhenium CO ₂ Reduction Catalysts Chemisorbed on SrTiO ₃ (100) Single Crystals. <i>Journal of Physical Chemistry C</i> , 2018, 122, 13944-13952. | 1.5 | 10 |
| 11692 | Determinant Role of Electrogenerated Reactive Nucleophilic Species on Selectivity during Reduction of CO ₂ Catalyzed by Metalloporphyrins. <i>Journal of the American Chemical Society</i> , 2018, 140, 4826-4834. | 6.6 | 75 |
| 11693 | Two luminescent transition-metal-organic frameworks with a pre-designed ligand as highly sensitive and selective iron(<i>iii</i>) sensors. <i>New Journal of Chemistry</i> , 2018, 42, 6839-6847. | 1.4 | 34 |
| 11694 | Experimental and computational evidence of halogen bonds involving astatine. <i>Nature Chemistry</i> , 2018, 10, 428-434. | 6.6 | 63 |
| 11695 | Polycyclic Aromatic Hydrocarbons with Straight Edges and the 7.6/6.2 and 8.6/6.2 Intensity Ratios in Reflection Nebulae. <i>Astrophysical Journal</i> , 2018, 854, 115. | 1.6 | 16 |
| 11696 | An Unprecedented Retro-Mumm Rearrangement Revealed by ESI-MS/MS, IRMPD Spectroscopy, and DFT Calculations. <i>Chemistry - A European Journal</i> , 2018, 24, 7026-7032. | 1.7 | 14 |
| 11697 | Histaminol and Its Complexes with Copper(II) - Studies in Solid State and Solution. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 1399-1408. | 1.0 | 13 |
| 11698 | Simulation and Analysis of the Spectroscopic Properties of Oxyluciferin and Its Analogues in Water. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2117-2126. | 2.3 | 32 |
| 11699 | Exploring the Chemoselective Dehydrogenative Silylation and Hydrogenation of Divinylsiloxane with Hydrosilane from DFT Computation. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 1993-1999. | 1.2 | 2 |
| 11700 | 1,2,4-Triazines in the Synthesis of Bipyridine Bisphenolate ONNO Ligands and Their Highly Luminescent Tetradentate Pt(II) Complexes for Solution-Processable OLEDs. <i>Inorganic Chemistry</i> , 2018, 57, 3825-3832. | 1.9 | 28 |
| 11701 | Highly selective iodide sensing ability of an anthraquinone-derived Schiff base in semi-aqueous medium and its performance in antioxidation, anti-inflammation and HRBC membrane protection. <i>New Journal of Chemistry</i> , 2018, 42, 6175-6182. | 1.4 | 6 |
| 11702 | Long-range corrected density functional through the density matrix expansion based semilocal exchange hole. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8991-8998. | 1.3 | 21 |
| 11703 | Mitochondria-localising DNA-binding biscyclometalated phenyltriazole iridium(III) dipyrrophenazine complexes: syntheses and cellular imaging properties. <i>Dalton Transactions</i> , 2018, 47, 4931-4940. | 1.6 | 16 |
| 11704 | Improved NOE fitting for flexible molecules based on molecular mechanics data – a case study with <i>S</i> -adenosylmethionine. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7523-7531. | 1.3 | 22 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11705 | Efficient implementation of one- and two-component analytical energy gradients in exact two-component theory. <i>Journal of Chemical Physics</i> , 2018, 148, 104110. | 1.2 | 56 |
| 11706 | Predictions of water/oil interfacial tension at elevated temperatures and pressures: A molecular dynamics simulation study with biomolecular force fields. <i>Fluid Phase Equilibria</i> , 2018, 476, 30-38. | 1.4 | 32 |
| 11707 | Infrared spectroscopy of isoprene in noble gas matrices. <i>Journal of Molecular Spectroscopy</i> , 2018, 348, 117-123. | 0.4 | 4 |
| 11708 | A Generalized Packing Model for Bulk Crystalline Regioregular Poly(3-alkylthiophenes) with Extended Side Chains. <i>Macromolecular Chemistry and Physics</i> , 2018, 219, 1700266. | 1.1 | 12 |
| 11709 | COSMO-based computer-aided molecular/mixture design: A focus on reaction solvents. <i>AIChE Journal</i> , 2018, 64, 104-122. | 1.8 | 39 |
| 11710 | Development of 4-hydrazinyl-7-nitrobenzofurazan as a fluorogenic probe for detecting malondialdehyde in biological samples. <i>Sensors and Actuators B: Chemical</i> , 2018, 254, 248-254. | 4.0 | 13 |
| 11711 | Low temperature kinetics and theoretical studies of the reaction $CN + CH_3NH_2$: a potential source of cyanamide and methyl cyanamide in the interstellar medium. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 5478-5489. | 1.3 | 33 |
| 11712 | Spin-Forbidden Reactions: Adiabatic Transition States Using Spin-Orbit Coupled Density Functional Theory. <i>Chemistry - A European Journal</i> , 2018, 24, 5006-5015. | 1.7 | 23 |
| 11713 | Spectroscopic investigations using density functional theory on 2-methoxy-4(phenyliminomethyl)phenol: A non linear optical material. <i>Journal of Molecular Structure</i> , 2018, 1155, 249-259. | 1.8 | 5 |
| 11714 | Dinuclear Iron(II) Spin-Crossover Compounds: A Theoretical Study. <i>Chemistry - A European Journal</i> , 2018, 24, 5183-5190. | 1.7 | 20 |
| 11715 | A reinvestigation of mono- and bis-ethynyl phosphonium salts: structural and computational studies and new reactivity. <i>Canadian Journal of Chemistry</i> , 2018, 96, 8-17. | 0.6 | 4 |
| 11716 | Synthesis, structural investigation and DFT studies on the intramolecular interaction in group 14 (2-CH ₃ OC ₆ H ₄)CH ₂ MPh ₃ (M = Si, Ge, Sn, Pb) organometallic compounds. <i>Inorganica Chimica Acta</i> , 2018, 475, 28-34. | 1.2 | 4 |
| 11717 | Crystal structures, vibrational spectra and DFT calculations of five halogeno-derivatives of 7-azaindole (3Br7AI, 4Br7AI, 4Cl7AI, 3Br4Cl7AI and 5Br3Cl7AI): a comparative study. <i>Journal of Molecular Structure</i> , 2018, 1152, 386-398. | 1.8 | 5 |
| 11718 | Aromatic hydrazones derived from nicotinic acid hydrazide as fluorimetric pH sensing molecules: Structural analysis by computational and spectroscopic methods in solid phase and in solution. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 190, 259-267. | 2.0 | 21 |
| 11719 | Theoretical studies on microstructures, stabilities and formation conditions of some sour gas in the type I, II, and H clathrate hydrates. <i>Journal of Molecular Structure</i> , 2018, 1153, 292-298. | 1.8 | 2 |
| 11720 | Mixed valent/geometry, linear, tetranuclear nickel complex bearing ONO pincer ligand exhibiting hitherto unknown ligation mode. <i>Polyhedron</i> , 2018, 143, 157-164. | 1.0 | 1 |
| 11721 | Interactions of Glycopolymers with Assemblies of Peptide Amphiphiles via Dynamic Covalent Bonding. <i>ACS Biomaterials Science and Engineering</i> , 2018, 4, 2061-2066. | 2.6 | 5 |
| 11722 | DFT computations on: Crystal structure, vibrational studies and optical investigations of a luminescent self-assembled material. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 191, 241-248. | 2.0 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11723 | Reactions of Sn(Si(Bu) ₂ Me) ₃ with HM(CO) ₃ CR ₅ (M = Cr or Mo, R = H or CH ₃) and Hg. Ionic, covalent, and $\frac{1}{4}$ -CO bonding patterns between transition metals and tin. <i>Inorganica Chimica Acta</i> , 2018, 469, 550-560. | 1.2 | 4 |
| 11724 | Reaction mechanism of chitosan/acrylamides dimer: A DFT study. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3775. | 0.9 | 4 |
| 11725 | Aluminum-poor hexacarbalane structures: The transition from localized organoaluminum structures to delocalized polyhedra. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25506. | 1.0 | 0 |
| 11726 | Synthesis and studies on gelation ability of phenol based maleate amphiphile and its application in nutraceutical release. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2018, 537, 310-317. | 2.3 | 6 |
| 11727 | Dual fluorescence of (E)-N-(4-(dimethylamino)benzylidene)-2H-1,2,4-triazol-3-amine (DMABA-Amtr): A ground state perspective. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 189, 601-607. | 2.0 | 3 |
| 11728 | Boron difluoride dibenzoylmethane derivatives: Electronic structure and luminescence. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 189, 563-570. | 2.0 | 12 |
| 11729 | Revised CHARMM force field parameters for iron-containing cofactors of photosystem II. <i>Journal of Computational Chemistry</i> , 2018, 39, 7-20. | 1.5 | 18 |
| 11730 | Computational study on the molecular conformations of phenolic compounds. <i>Structural Chemistry</i> , 2018, 29, 179-194. | 1.0 | 11 |
| 11731 | Structures and thermochemistry of methyl ethyl sulfide and its hydroperoxides: HOOCH ₂ SCH ₂ CH ₃ , CH ₃ SCH(OOH)CH ₃ , CH ₃ SCH ₂ CH ₂ OOH, and radicals. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3751. | 0.9 | 4 |
| 11732 | Preparation and characterization by infrared emission spectroscopy and applications of new mineral-based composite materials of biomedical interest. <i>Applied Spectroscopy Reviews</i> , 2018, 53, 439-485. | 3.4 | 1 |
| 11733 | Noncovalent interactions between cisplatin and graphene prototypes. <i>Journal of Computational Chemistry</i> , 2018, 39, 71-80. | 1.5 | 13 |
| 11734 | Development of new selective ethylene trimerization catalysts based on highly active ethylene polymerization catalysts. <i>Catalysis Today</i> , 2018, 303, 263-270. | 2.2 | 7 |
| 11735 | Water-insoluble cyclodextrin membranes for humidity detection: green synthesis, characterization and sensing performances. <i>Journal of Materials Science</i> , 2018, 53, 1455-1469. | 1.7 | 10 |
| 11736 | DFT studies on the ligand effect on electronic and optical properties of three series of functionalized Ir(III) complexes. <i>Journal of Molecular Structure</i> , 2018, 1151, 49-55. | 1.8 | 0 |
| 11737 | Kinetics and mechanistic study of polynuclear platinum(II) polypyridyl complexes; A paradigm shift in search of new anticancer agents. <i>Inorganica Chimica Acta</i> , 2018, 469, 341-352. | 1.2 | 8 |
| 11738 | The not-so-simple coordination chemistry of alkali-metal cations Li ⁺ , Na ⁺ and K ⁺ with one carbonate anion: A study using density functional and atoms in molecules theories. <i>Inorganica Chimica Acta</i> , 2018, 469, 245-254. | 1.2 | 3 |
| 11739 | Electronic structure and reactivity studies of a nonsymmetric one-electron oxidized CuII bis-phenoxide complex. <i>Inorganica Chimica Acta</i> , 2018, 481, 151-158. | 1.2 | 8 |
| 11740 | Preparation of a coordinatively saturated $\frac{1}{4}$ - $\frac{1}{2}$ -peroxodicopper(II) compound. <i>Inorganica Chimica Acta</i> , 2018, 481, 166-170. | 1.2 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11741 | Construction of one dimensional Co(II) and Zn(II) coordination polymers based on expanded N,N- π -donor ligands. <i>Inorganica Chimica Acta</i> , 2018, 469, 461-468. | 1.2 | 8 |
| 11742 | Organic-inorganic hybrid materials from divalent metal cations and expanded N,N- π -donor linkers. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2018, 233, 97-111. | 0.4 | 1 |
| 11743 | Synthesis, photophysical properties and cation-binding studies of bipyridine-functionalized gold(κ) complexes. <i>Inorganic Chemistry Frontiers</i> , 2018, 5, 160-171. | 3.0 | 18 |
| 11744 | Benzimidazobenzothiazole-based highly-efficient thermally activated delayed fluorescence emitters for organic light-emitting diodes: A quantum-chemical TD-DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 192, 297-303. | 2.0 | 5 |
| 11745 | An improved two-rotor function for conformational potential energy surfaces of 20 amino acid diamides. <i>Canadian Journal of Chemistry</i> , 2018, 96, 58-71. | 0.6 | 2 |
| 11746 | Thermodynamics of aqueous perfluorooctanoic acid (PFOA) and 4,8-dioxo-3H-perfluorononanoic acid (DONA) from DFT calculations: Insights into degradation initiation. <i>Chemosphere</i> , 2018, 193, 1063-1070. | 4.2 | 20 |
| 11747 | New luminescent copper(I) complexes with extended π -conjugation. <i>Polyhedron</i> , 2018, 140, 42-50. | 1.0 | 18 |
| 11748 | From bismuth oxide/hydroxide precursor clusters towards stable oxides: Proton transfer reactions and structural reorganization govern the stability of [Bi ₁₈ O ₁₃ (OH) ₁₀]-nitrate clusters. <i>Chemical Physics Letters</i> , 2018, 691, 87-90. | 1.2 | 3 |
| 11749 | Spectroscopic and theoretical studies of dalbergin and Methylalbergin. <i>Journal of Molecular Structure</i> , 2018, 1156, 243-254. | 1.8 | 4 |
| 11750 | Quantum yield improvement of red-light-emitting firefly luciferin analogues for in vivo bioluminescence imaging. <i>Tetrahedron</i> , 2018, 74, 652-660. | 1.0 | 25 |
| 11751 | Reversible piezochromic luminescence of coumarin hydrozone derivatives and the influence of substituents. <i>Journal of Luminescence</i> , 2018, 195, 126-133. | 1.5 | 3 |
| 11752 | Unusual response to environmental polarity in a nonlinear-optical benzylidene-type chromophore containing a 1,3-bis(dicyanomethylidene)indane acceptor fragment. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 404-413. | 1.3 | 5 |
| 11753 | Mechanistic insights into the catalytic carbonyl hydrosilylation by cationic [CpM(CO) ₂ (IMes)] ⁺ (M = Mo, W) complexes: the intermediacy of η -H(Si) metal complexes. <i>New Journal of Chemistry</i> , 2018, 42, 4923-4932. | 1.4 | 5 |
| 11754 | Theoretical investigation of the impact of ligands on the regiodivergent Rh-catalyzed hydrothiolation of allyl amines. <i>Dalton Transactions</i> , 2018, 47, 150-158. | 1.6 | 21 |
| 11755 | Mapping the 3D orientation of piconewton integrin traction forces. <i>Nature Methods</i> , 2018, 15, 115-118. | 9.0 | 105 |
| 11756 | How accurate is the description of ligand-protein interactions by a hybrid QM/MM approach?. <i>Journal of Molecular Modeling</i> , 2018, 24, 11. | 0.8 | 19 |
| 11757 | Captodative Substitution: A Strategy for Enhancing the Conductivity of Molecular Electronic Devices. <i>Journal of Physical Chemistry C</i> , 2018, 122, 3194-3200. | 1.5 | 32 |
| 11758 | Heterometallic boride clusters: synthesis and characterization of butterfly and square pyramidal boride clusters*. <i>Pure and Applied Chemistry</i> , 2018, 90, 665-675. | 0.9 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11759 | The Reactivity of Cyameluric Chloride $C_6N_7Cl_3$ towards Phosphines and Phosphine Oxides. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2018, 644, 121-126. | 0.6 | 8 |
| 11760 | Corrected Polarizable Embedding: Improving the Induction Contribution to Perichromism for Linear Response Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 833-842. | 2.3 | 12 |
| 11761 | Dibenzo[<i>a,e</i>]pentalenes with Low-Lying LUMO Energy Levels as Potential n-Type Materials. <i>Journal of Organic Chemistry</i> , 2018, 83, 656-663. | 1.7 | 40 |
| 11762 | How to tame a palladium terminal oxo. <i>Chemical Science</i> , 2018, 9, 1155-1167. | 3.7 | 24 |
| 11763 | Theoretical study on photo-induced processes of 1-methyl-3-(1,8-naphthalimidyl)ethylimidazolium halide species: an application of constrained density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3911-3917. | 1.3 | 5 |
| 11764 | Pure white light emission from a rare earth-free intrinsic metal-organic framework and its application in a WLED. <i>Journal of Materials Chemistry C</i> , 2018, 6, 614-621. | 2.7 | 53 |
| 11765 | Conformational switching <i>via</i> an intramolecular H-bond modulates the fluorescence lifetime in a novel coumarin-imidazole conjugate. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6060-6072. | 1.3 | 10 |
| 11766 | Sequential <i>meta-ortho</i> -C-H Functionalizations by One-Pot Ruthenium(II/III) Catalysis. <i>ACS Catalysis</i> , 2018, 8, 886-892. | 5.5 | 115 |
| 11767 | The coordination- and photochemistry of copper complexes: variation of N ligands from imidazole to tetrazole. <i>Dalton Transactions</i> , 2018, 47, 608-621. | 1.6 | 47 |
| 11768 | Metal-metal bonding in deltahedral dimetallaboranes and trimetallaboranes: a density functional theory study. <i>Pure and Applied Chemistry</i> , 2018, 90, 643-652. | 0.9 | 0 |
| 11769 | Aluminum Atom Activation of C-S Bonds: An EPR Study of the Intermediates Formed in the Reaction Between Aluminum Atoms and Dialkyl Sulfides. <i>Journal of Physical Chemistry A</i> , 2018, 122, 72-80. | 1.1 | 2 |
| 11770 | Theoretical study of the reactions of the hydroselenyl radical (HSe \cdot) with the selenenic radical (HSeO \cdot). <i>Journal of Molecular Modeling</i> , 2018, 24, 3. | 0.8 | 0 |
| 11771 | Analysis of the conformational properties of amine ligands at the gold/water interface with QM, MM and QM/MM simulations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3349-3362. | 1.3 | 15 |
| 11772 | Hidden in Condensed State Solvation: Multiradiative Channels Design for Highly Efficient Solution-Processed Purely Organic Electroluminescence at High Brightness. <i>Advanced Functional Materials</i> , 2018, 28, 1704927. | 7.8 | 105 |
| 11773 | The Eponymous Cofactors in Cytochrome P460s from Ammonia-Oxidizing Bacteria Are Iron Porphyrinoids Whose Macrocycles Are Dibasic. <i>Biochemistry</i> , 2018, 57, 334-343. | 1.2 | 12 |
| 11774 | Understanding and Breaking Scaling Relations in Single-Site Catalysis: Methane to Methanol Conversion by $Fe^{IV}=\text{O}$. <i>ACS Catalysis</i> , 2018, 8, 975-986. | 5.5 | 119 |
| 11775 | Electrocatalytic Reduction of Dioxygen to Hydrogen Peroxide by a Molecular Manganese Complex with a Bipyridine-Containing Schiff Base Ligand. <i>Journal of the American Chemical Society</i> , 2018, 140, 3232-3241. | 6.6 | 56 |
| 11776 | X-Shaped Oligomeric Pyromellitimide Polyradicals. <i>Journal of the American Chemical Society</i> , 2018, 140, 515-523. | 6.6 | 15 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11777 | Fiber enhanced Raman sensing of levofloxacin by PCF bandgap-shifting into the visible range. <i>Analytical Methods</i> , 2018, 10, 586-592. | 1.3 | 36 |
| 11778 | Computerchemie: das Schicksal aktueller Methoden und zukünftige Herausforderungen. <i>Angewandte Chemie</i> , 2018, 130, 4241-4248. | 1.6 | 16 |
| 11779 | Computational Chemistry: The Fate of Current Methods and Future Challenges. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 4170-4176. | 7.2 | 138 |
| 11780 | Mechanistic insight into the C7-selective C-H functionalization of <i>N</i> -acyl indole catalyzed by a rhodium complex: a theoretical study. <i>Organic Chemistry Frontiers</i> , 2018, 5, 725-733. | 2.3 | 25 |
| 11781 | Accuracy of dielectric-dependent hybrid functionals in the prediction of optoelectronic properties of metal oxide semiconductors: a comprehensive comparison with many-body GW and experiments. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 044003. | 0.7 | 59 |
| 11782 | Conceptual Insights into DFT Spin-State Energetics of Octahedral Transition-Metal Complexes through a Density Difference Analysis. <i>Chemistry - A European Journal</i> , 2018, 24, 5281-5292. | 1.7 | 34 |
| 11783 | Frontiers of Coupled Cluster Chiroptical Response Theory. , 2018, , 49-68. | | 3 |
| 11784 | Rapid and simultaneous synthesis of a hydrogen bond templated [3]rotaxane and its related [2]rotaxane molecular shuttle. <i>Supramolecular Chemistry</i> , 2018, 30, 758-764. | 1.5 | 10 |
| 11785 | Correlating the vibrational spectra of structurally related molecules: A spectroscopic measure of similarity. <i>Journal of Computational Chemistry</i> , 2018, 39, 293-306. | 1.5 | 11 |
| 11786 | Design of zinc porphyrin- <i>perylene</i> diimide donor-bridge-acceptor chromophores for large second-order nonlinear optical response: A theoretical exploration. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25536. | 1.0 | 10 |
| 11787 | A computational investigation into nickel-bis(diselenolene) complexes as potential catalysts for reduction of H ⁺ to H ₂ . <i>Canadian Journal of Chemistry</i> , 2018, 96, 51-57. | 0.6 | 3 |
| 11788 | Distal Weak Coordination of Acetamides in Ruthenium(II)-Catalyzed C-H Activation Processes. <i>Angewandte Chemie</i> , 2018, 130, 773-776. | 1.6 | 22 |
| 11789 | Substituent effects in the Nicholas epimerization of glycosides. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3780. | 0.9 | 3 |
| 11790 | Rare-earth metal-mediated PhC ₆ N insertion into <i>N,N</i> -bis(trimethylsilyl)naphthalene-1,8-diamido dianion - a synthetic approach to complexes coordinated by <i>ansa</i> -bridged amido-amidinato ligand. <i>Dalton Transactions</i> , 2018, 47, 438-451. | 1.6 | 4 |
| 11791 | Impact of Substituent Variation on the Presence of Thermal Spin Crossover in a Series of Mononuclear Iron(III) Schiff Base Complexes with Terminal Pseudohalido Co-ligands. <i>Chemistry - A European Journal</i> , 2018, 24, 5191-5203. | 1.7 | 15 |
| 11792 | Identification of initial decomposition reactions in liquid-phase HMX using quantum mechanics calculations. <i>Combustion and Flame</i> , 2018, 188, 170-179. | 2.8 | 20 |
| 11793 | Mechanistic study on the Rh(III)-catalyzed synthesis of indolines via selective O-atom transfer of aryl nitrones: Origins of the regioselectivity and the improved yield with pivalic acid additive. <i>Journal of Organometallic Chemistry</i> , 2018, 854, 15-26. | 0.8 | 7 |
| 11794 | Structural characterizations, Hirshfeld surface analyses, and third-order nonlinear optical properties of two novel chalcone derivatives. <i>Optical Materials</i> , 2018, 75, 580-594. | 1.7 | 85 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11795 | Performance of density functionals for modeling vapor liquid equilibria of CO ₂ and SO ₂ . <i>Journal of Computational Chemistry</i> , 2018, 39, 397-406. | 1.5 | 12 |
| 11796 | Additional donor bridge as a design approach for multi-anchoring dyes for highly efficient dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 352, 86-97. | 2.0 | 19 |
| 11797 | Dispersion corrected density functional study of CO oxidation on pristine/functionalized/doped graphene surfaces in aqueous phase. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 79, 27-34. | 1.3 | 5 |
| 11798 | A novel coumarin-pyrazole-triazine based fluorescence chemosensor for fluoride detection via deprotonation process: Experimental and theoretical studies. <i>Journal of Molecular Structure</i> , 2018, 1155, 573-581. | 1.8 | 15 |
| 11799 | Redox-Dependent Metal-Metal Bonding in Trinuclear Metal Chains: Probing the Transition from Covalent Bonding to Exchange Coupling. <i>Chemistry - A European Journal</i> , 2018, 24, 5309-5318. | 1.7 | 2 |
| 11800 | Density functional theory study on the dihydrogen bond cooperativity in the growth behavior of dimethyl sulfoxide clusters. <i>Journal of Molecular Liquids</i> , 2018, 249, 454-462. | 2.3 | 30 |
| 11801 | Dynamics of H ₂ O ligands and ReO ₄ ⁻ anions at the phase transition in [Mn(H ₂ O) ₂](ReO ₄) ₂ studied by complementary spectroscopic methods. <i>Journal of Raman Spectroscopy</i> , 2018, 49, 298-311. | 1.2 | 4 |
| 11802 | Design and synthesis of new thiobarbituric acid metal complexes as potent protease inhibitors: spectral characterization, thermal analysis and DFT calculations. <i>Journal of the Iranian Chemical Society</i> , 2018, 15, 269-280. | 1.2 | 8 |
| 11803 | Ab initio calculations of open cell voltage in newly designed PTMA-based Li-ion organic radical batteries. <i>Computational Materials Science</i> , 2018, 143, 27-31. | 1.4 | 4 |
| 11804 | Effect of asphaltene dispersion on slurry-phase hydrocracking of heavy residual hydrocarbons. <i>Fuel</i> , 2018, 214, 174-186. | 3.4 | 22 |
| 11805 | Distal Weak Coordination of Acetamides in Ruthenium(II)-Catalyzed C-H Activation Processes. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 765-768. | 7.2 | 83 |
| 11806 | Three-Component Synthesis and Photophysical Properties of Novel Coumarin-Based Merocyanines. <i>Chemistry - A European Journal</i> , 2018, 24, 974-983. | 1.7 | 27 |
| 11807 | An oxorhenium complex bearing a chiral cyclohexane-1,2-ethiolato ligand: Synthesis, stereochemistry, and theoretical study of parity violation vibrational frequency shifts. <i>Chirality</i> , 2018, 30, 147-156. | 1.3 | 6 |
| 11808 | The effect of alkyl chain tethers on the kinetics and mechanistic behaviour of bifunctional dinuclear platinum(II) complexes bearing 1,2-dipyridylamine ligands. <i>New Journal of Chemistry</i> , 2018, 42, 214-227. | 1.4 | 7 |
| 11809 | A [HN(BH ₂) ₂] ²⁻ Dianion, Isoelectronic with a ²⁻ -Diketimate. <i>Organometallics</i> , 2018, 37, 628-631. | 1.1 | 4 |
| 11810 | The mechanism of the reaction between an aziridine and carbon dioxide with no added catalyst. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3735. | 0.9 | 14 |
| 11811 | Combined plane wave and localized orbital electronic structure calculation: Adsorption energy of hydrogen on Pd(111). <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25452. | 1.0 | 5 |
| 11812 | Absorption mechanism, structural and electronic properties of MC19 (M = B and Si) fullerenes with 1-acetylpiperazine. <i>Adsorption Science and Technology</i> , 2018, 36, 797-804. | 1.5 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11813 | Effectiveness of Complex Esters According to the Integral Criterion of Molecular Electronegativity in the Flotation of Gas Coal. <i>Coke and Chemistry</i> , 2018, 61, 413-418. | 0.0 | 1 |
| 11814 | Quantum-Chemical Study of the Adsorption of Bi ³⁺ Ions on Au(111). <i>Russian Journal of Electrochemistry</i> , 2018, 54, 1201-1208. | 0.3 | 1 |
| 11815 | Identification of structural criteria for valence state localization in linear alkanes. , 2018, , . | | 1 |
| 11816 | Quantum-Chemical Study of the Adsorption of Pb ²⁺ on Au(111). <i>Russian Journal of Electrochemistry</i> , 2018, 54, 902-911. | 0.3 | 2 |
| 11817 | Interaction between Thallium and the Au(111) Surface. Quantum-Chemical Analysis. <i>Russian Journal of Electrochemistry</i> , 2018, 54, 912-921. | 0.3 | 0 |
| 11819 | Diversity-Oriented Synthesis and Optical Properties of Bichromophoric Pyrrole-Fluorophore Conjugates. <i>Frontiers in Chemistry</i> , 2018, 6, 579. | 1.8 | 4 |
| 11820 | Liquid-Phase Hydrogenation of Halobenzenes in the Presence of Palladium-Containing Nanodiamonds. <i>Petroleum Chemistry</i> , 2018, 58, 1206-1212. | 0.4 | 3 |
| 11821 | An improved descriptor of cluster stability: application to small carbon clusters. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27368-27374. | 1.3 | 8 |
| 11822 | Effect of the degree of inversion on optical properties of spinel ZnFe ₂ O ₄ . <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28267-28278. | 1.3 | 88 |
| 11823 | Reactions of dicobalt octacarbonyl with dinucleating and mononucleating bis(imino)pyridine ligands. <i>Dalton Transactions</i> , 2018, 47, 15353-15363. | 1.6 | 17 |
| 11824 | 3D isomorphous lanthanide coordination polymers displaying magnetic refrigeration, slow magnetic relaxation and tunable proton conduction. <i>Dalton Transactions</i> , 2018, 47, 15405-15415. | 1.6 | 48 |
| 11825 | Electronic properties of the coronene series from thermally-assisted-occupation density functional theory. <i>RSC Advances</i> , 2018, 8, 34350-34358. | 1.7 | 21 |
| 11826 | Reaction of FcC≡CC(O)R (Fc = ferrocenyl) with Ru ₃ (CO) ₁₂ leading to unexpected nitro-group reduced ruthenoles and 1,2-CO-inserted triruthenium clusters. <i>RSC Advances</i> , 2018, 8, 25268-25276. | 1.7 | 4 |
| 11827 | Click 1,2,3-triazole derived fluorescent scaffold by mesoionic carbene-nitrene cyclization: an experimental and theoretical study. <i>New Journal of Chemistry</i> , 2018, 42, 18969-18978. | 1.4 | 5 |
| 11828 | Deprotonated carbohydrate anion fragmentation chemistry: structural evidence from tandem mass spectrometry, infra-red spectroscopy, and theory. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27897-27909. | 1.3 | 19 |
| 11829 | Unveiling the role of intra and interatomic interactions in the energetics of reaction schemes: a quantum chemical topology analysis. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27558-27570. | 1.3 | 5 |
| 11830 | Understanding interactions of organic nitrates with the surface and bulk of organic films: implications for particle growth in the atmosphere. <i>Environmental Sciences: Processes and Impacts</i> , 2018, 20, 1593-1610. | 1.7 | 12 |
| 11831 | Tunable ESIPT reaction and antioxidant activities of 3-hydroxyflavone and its derivatives by altering atomic electronegativity. <i>Organic Chemistry Frontiers</i> , 2018, 5, 3435-3442. | 2.3 | 76 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11832 | Influence of odd-even effect and intermolecular interactions in 2D molecular layers of bisamide organogelators. <i>RSC Advances</i> , 2018, 8, 35195-35204. | 1.7 | 7 |
| 11833 | Multiple 3D-QSAR modeling, e-pharmacophore, molecular docking, and <i>in vitro</i> study to explore novel AChE inhibitors. <i>RSC Advances</i> , 2018, 8, 39477-39495. | 1.7 | 36 |
| 11834 | Identification of structural criteria for valence state localization in linear alkanes. , 2018, , . | | 1 |
| 11835 | Inverted solvatochromic Stokes shift in GFP-like chromophores with extended conjugation. <i>Chinese Journal of Chemical Physics</i> , 2018, 31, 599-607. | 0.6 | 0 |
| 11836 | Study on the Mechanism of Cold and Negative Temperature Coefficient in Natural Process of Gasoline Hydrocarbon. <i>MATEC Web of Conferences</i> , 2018, 166, 02007. | 0.1 | 0 |
| 11837 | Interplay between test sets and statistical procedures in ranking DFT methods: The case of electron density studies. <i>Mendeleev Communications</i> , 2018, 28, 225-235. | 0.6 | 36 |
| 11838 | Computational Exploration of a Pd(II)-Catalyzed \hat{I}^3 -C-H Arylation Where Stereoselectivity Arises from Attractive Aryl-Aryl Interactions. <i>Journal of Organic Chemistry</i> , 2018, 83, 14786-14790. | 1.7 | 8 |
| 11839 | Fundamental Gaps of Condensed-Phase Organic Semiconductors from Single-Molecule Calculations using Polarization-Consistent Optimally Tuned Screened Range-Separated Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6287-6294. | 2.3 | 76 |
| 11840 | Origin of the \hat{I}^3 -Spacing Change upon Doping of Semiconducting Polymers. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27983-27990. | 1.5 | 25 |
| 11841 | Can Adsorption on Graphene be Used for Isotopic Enrichment? A DFT Perspective. <i>Molecules</i> , 2018, 23, 2981. | 1.7 | 7 |
| 11842 | Calcium-Induced Lipid Nanocluster Structures: Sculpturing of the Plasma Membrane. <i>Biochemistry</i> , 2018, 57, 6897-6905. | 1.2 | 14 |
| 11843 | All-Thiophene-Based Double Helix: Synthesis, Crystal Structure, Chiroptical Property and Arylation. <i>ACS Omega</i> , 2018, 3, 16014-16020. | 1.6 | 6 |
| 11844 | Ambimodal Dipolar/Diels-Alder Cycloaddition Transition States Involving Proton Transfers. <i>Journal of the American Chemical Society</i> , 2018, 140, 18124-18131. | 6.6 | 26 |
| 11845 | A series of 1-D zinc(II) coordination polymers with 3-D supramolecular networks: synthesis, structural investigation, and NBO analysis. <i>Journal of Coordination Chemistry</i> , 2018, 71, 4031-4046. | 0.8 | 0 |
| 11846 | Mechanisms of Bisphosphine Iron-Catalyzed C(SP ²)-C(SP ³) Cross-Coupling Reactions: Inner-Sphere or Outer-Sphere Arylation?. <i>Comments on Inorganic Chemistry</i> , 2018, 38, 210-237. | 3.0 | 8 |
| 11847 | Understanding structure-activity relationships in linear polymer photocatalysts for hydrogen evolution. <i>Nature Communications</i> , 2018, 9, 4968. | 5.8 | 244 |
| 11848 | Structure of Active Sites of Fe-N-C Nano-Catalysts for Alkaline Exchange Membrane Fuel Cells. <i>Nanomaterials</i> , 2018, 8, 965. | 1.9 | 13 |
| 11849 | Complexation of Ca ²⁺ cation by the lateral chain of Paclitaxel (N-Benzoyl- \hat{Y} -phenylisoserine): A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2018, 1146, 1-9. | 1.1 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11850 | Differential Stabilization of the Metal–Ligand Complexes between Organic and Aqueous Phases Drives the Selectivity of Phosphoric Acid Ligands toward Heavier Rare Earth Elements. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 17209-17217. | 1.8 | 7 |
| 11851 | Complementary Quantitative Structure–Activity Relationship Models for the Antitrypanosomal Activity of Sesquiterpene Lactones. <i>International Journal of Molecular Sciences</i> , 2018, 19, 3721. | 1.8 | 11 |
| 11852 | New Acridine-Based Tridentate Ligand for Ruthenium(II): Coordination with a Twist. <i>Inorganic Chemistry</i> , 2018, 57, 15430-15437. | 1.9 | 9 |
| 11853 | QSAR and Molecular Docking Studies of the Inhibitory Activity of Novel Heterocyclic GABA Analogues over GABA-AT. <i>Molecules</i> , 2018, 23, 2984. | 1.7 | 7 |
| 11854 | Shrinking Self-Interaction Errors with the Fermi–Lindin Orbital Self-Interaction-Corrected Density Functional Approximation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9307-9315. | 1.1 | 30 |
| 11855 | Impact of Ferrocene Substitution on the Electronic Properties of BODIPY Derivatives and Analogues. <i>Inorganic Chemistry</i> , 2018, 57, 14698-14704. | 1.9 | 6 |
| 11856 | Quantum-chemical modelling of clay mineral surfaces and clay mineral–surface–adsorbate interactions. <i>Developments in Clay Science</i> , 2018, 9, 49-87. | 0.3 | 7 |
| 11857 | Improving the Global Electrophilicity Index (GEI) as a Measure of Lewis Acidity. <i>Inorganic Chemistry</i> , 2018, 57, 14764-14771. | 1.9 | 65 |
| 11858 | Ruthenium(II) Bipyridyl Complexes with C ^{≡S} C* Cyclometalated Mesoionic Carbene Ligands. <i>Organometallics</i> , 2018, 37, 4619-4629. | 1.1 | 16 |
| 11859 | Low scaling EOM-CCSD and EOM-MBPT(2) method with natural transition orbitals. <i>Journal of Chemical Physics</i> , 2018, 149, 184103. | 1.2 | 14 |
| 11860 | An efficient first principles method for molecular pump-probe NEXAFS spectra: Application to thymine and azobenzene. <i>Journal of Chemical Physics</i> , 2018, 149, 144112. | 1.2 | 21 |
| 11861 | Raman and Computational Study on the Adsorption of Xanthine on Silver Nanocolloids. <i>ACS Omega</i> , 2018, 3, 13530-13537. | 1.6 | 16 |
| 11862 | Gaussian process based optimization of molecular geometries using statistically sampled energy surfaces from quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2018, 149, 164116. | 1.2 | 10 |
| 11863 | Structural evolution and bonding properties of BSi ⁿ / (n = 4–12) clusters: Size-selected anion photoelectron spectroscopy and theoretical calculations. <i>Journal of Chemical Physics</i> , 2018, 149, 174314. | 1.2 | 17 |
| 11864 | Synthesis, Characterization and Electronic Structure of Dirhenadehydro[12]annulene Complexes. <i>ChemPlusChem</i> , 2019, 84, 85-91. | 1.3 | 7 |
| 11865 | Cloud Automation to Run Large-Scale Quantum Chemical Simulations. , 2018, , . | | 0 |
| 11866 | Communication: Becke's virial exciton model gives accurate charge-transfer excitation energies. <i>Journal of Chemical Physics</i> , 2018, 149, 231101. | 1.2 | 9 |
| 11867 | Sensing Performance and Efficiency of Two Energy Transfer-Based Two-Photon Fluorescent Probes for pH. <i>Sensors</i> , 2018, 18, 4407. | 2.1 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11868 | A Density Functional Theory Study on the Acid-Catalyzed Transesterification Mechanism for Biodiesel Production from Waste Cooking Oils. <i>JAOCS, Journal of the American Oil Chemists' Society</i> , 2019, 96, 137-145. | 0.8 | 5 |
| 11869 | First principles calculation of spin-related quantities for point defect qubit research. <i>Npj Computational Materials</i> , 2018, 4, . | 3.5 | 56 |
| 11871 | Computational Prediction of Electronic and Photovoltaic Properties of Anthracene-Based Organic Dyes for Dye-Sensitized Solar Cells. <i>International Journal of Photoenergy</i> , 2018, 2018, 1-17. | 1.4 | 2 |
| 11872 | Role of TiO ₂ Anatase Surface Morphology on Organophosphorus Interfacial Chemistry. <i>Journal of Physical Chemistry C</i> , 2018, 122, 29237-29248. | 1.5 | 16 |
| 11873 | Theoretical Approaches to Describing the Oxygen Reduction Reaction Activity of Single-Atom Catalysts. <i>Journal of Physical Chemistry C</i> , 2018, 122, 29307-29318. | 1.5 | 68 |
| 11874 | Demystifying Cp ₂ Ti(H)Cl and Its Enigmatic Role in the Reactions of Epoxides with Cp ₂ TiCl. <i>Organometallics</i> , 2018, 37, 4801-4809. | 1.1 | 32 |
| 11875 | On the geometric dependence of the molecular dipole polarizability in water: A benchmark study of higher-order electron correlation, basis set incompleteness error, core electron effects, and zero-point vibrational contributions. <i>Journal of Chemical Physics</i> , 2018, 149, 204303. | 1.2 | 11 |
| 11876 | New Aryl-Substituted 2,2'-Bithiophenes: Synthesis, Optoelectronic Properties and DFT Studies. <i>ChemistrySelect</i> , 2018, 3, 9700-9707. | 0.7 | 0 |
| 11877 | Structural, Optical, and Magnetic Properties of Ultramarine Pigments: A DFT Insight. <i>Journal of Physical Chemistry C</i> , 2018, 122, 29338-29349. | 1.5 | 8 |
| 11878 | Electron paramagnetic resonance study of Gabapentin and Pregabalin molecules with density functional theory. <i>AIP Conference Proceedings</i> , 2018, . | 0.3 | 1 |
| 11879 | Sequence Ion Structures and Dissociation Chemistry of Deprotonated Sucrose Anions. <i>Journal of the American Society for Mass Spectrometry</i> , 2018, 29, 2380-2393. | 1.2 | 15 |
| 11880 | A DFT prediction on the chemical reactivity of novel azoethione derivatives as chelating agents: Implications for copper minerals flotation and copper corrosion inhibition. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2018, 93, 109-123. | 2.7 | 45 |
| 11881 | A theoretical investigation of the reaction between the amidogen, NH, and the ethyl, C ₂ H ₅ , radicals: a possible gas-phase formation route of interstellar and planetary ethanimine. <i>Molecular Astrophysics</i> , 2018, 13, 30-37. | 1.7 | 24 |
| 11882 | Solvation of Piperidine in Nonaqueous Solvents. <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 2095-2097. | 0.1 | 1 |
| 11883 | On the many-electron self-interaction error of the semilocal exchange hole based meta-GGA level range-separated hybrid with the B88 hybrids. <i>Chemical Physics Letters</i> , 2018, 713, 1-9. | 1.2 | 17 |
| 11884 | Strategies and Software for Machine Learning Accelerated Discovery in Transition Metal Chemistry. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 13973-13986. | 1.8 | 104 |
| 11885 | Analysis of two [2]catenanes based on electron densities from invariom refinement and results from DFT calculations. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2018, 73, 677-687. | 0.3 | 3 |
| 11886 | The Light-Driven Isomerization of Aqueous Nitrate: A Theoretical Perspective. <i>ChemPhotoChem</i> , 2018, 2, 725-733. | 1.5 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11887 | On the nature of the boron–copper interaction. Topological study of the electron localisation function (ELF). <i>New Journal of Chemistry</i> , 2018, 42, 17096-17114. | 1.4 | 5 |
| 11888 | Efficient lattice constants and energy bandgaps for condensed systems from a meta-GGA level screened range-separated hybrid functional. <i>Journal of Chemical Physics</i> , 2018, 149, 094105. | 1.2 | 14 |
| 11889 | Auger electron angular distributions following excitation or ionization of the I 3d level in methyl iodide. <i>Journal of Chemical Physics</i> , 2018, 149, 094304. | 1.2 | 11 |
| 11890 | Characterizing self-assembled molecular layers on weakly interacting substrates: the role of van der Waals and the chemical interactions. <i>Nano Futures</i> , 2018, 2, 045002. | 1.0 | 2 |
| 11891 | Synthesis and Characterization of Readily Modified Poly(aryl)(alkoxy)stannanes by use of Hypercoordinated Sn Monomers. <i>Chemistry - A European Journal</i> , 2018, 24, 18762-18771. | 1.7 | 8 |
| 11892 | Towards hybrid density functional calculations of molecular crystals via fragment-based methods. <i>Journal of Chemical Physics</i> , 2018, 149, 124104. | 1.2 | 13 |
| 11893 | Computational study of Rh(I)-Catalyzed Cycloaddition–Fragmentation of N-cyclopropylacrylamides. <i>Tetrahedron</i> , 2018, 74, 6475-6483. | 1.0 | 2 |
| 11894 | Ligand Exchange Reaction on a Ru(II)–Pheox Complex as a Mechanistic Study of Catalytic Reactions. <i>ACS Omega</i> , 2018, 3, 11286-11289. | 1.6 | 10 |
| 11895 | Molecular Dynamics Simulations of the Interactions between Glial Cell Line-Derived Neurotrophic Factor Family Receptor GFR α 1 and Small-Molecule Ligands. <i>ACS Omega</i> , 2018, 3, 11407-11414. | 1.6 | 69 |
| 11896 | Synthesis, Crystal Structures and Magnetic Properties of Two Heterobridged μ -Phenoxo- μ -1,1-Azide/Isocyanate Dinickel(II) Compounds: Experimental and Theoretical Exploration. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 4556-4565. | 1.0 | 11 |
| 11897 | Theoretical Study of the Copper-Catalyzed Hydroarylation of (Trifluoromethyl)alkyne with Phenylboronic Acid. <i>Journal of Organic Chemistry</i> , 2018, 83, 12775-12783. | 1.7 | 11 |
| 11898 | Introduction to modeling nanoclusters and nanoparticles. <i>Frontiers of Nanoscience</i> , 2018, 12, 1-54. | 0.3 | 4 |
| 11899 | X-ray Raman scattering: a new <i>in situ</i> probe of molecular structure during nucleation and crystallization from liquid solutions. <i>CrystEngComm</i> , 2018, 20, 6871-6884. | 1.3 | 8 |
| 11900 | Umbrella inversion and structure of phosphorus-containing compounds: A quantum chemical study. <i>Journal of Theoretical and Computational Chemistry</i> , 2018, 17, 1850042. | 1.8 | 7 |
| 11901 | <i>P</i> , <i>P</i> -Dimethylformylphosphine: The Phosphorus Analogue of <i>N</i> , <i>N</i> -Dimethylformamide. <i>Journal of the American Chemical Society</i> , 2018, 140, 12751-12755. | 6.6 | 19 |
| 11902 | Uncontracted core Pople basis sets in vibrational frequency calculations. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25761. | 1.0 | 4 |
| 11903 | Electronic structure and photoelectron spectroscopy of manganese dihalides from quantum chemical methods and Dyson orbitals. <i>Chemical Physics</i> , 2018, 515, 513-520. | 0.9 | 2 |
| 11904 | Silver(I)-Catalyzed C–X, C–C, C–N, and C–O Cross-Couplings Using Aminoquinoline Directing Group via Elusive Aryl-Ag(III) Species. <i>ACS Catalysis</i> , 2018, 8, 10430-10436. | 5.5 | 27 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 11905 | Sulfone-containing covalent organic frameworks for photocatalytic hydrogen evolution from water. <i>Nature Chemistry</i> , 2018, 10, 1180-1189. | 6.6 | 883 |
| 11906 | Chiral Control in Pentacoordinate Systems: The Case of Organosilicates. <i>Inorganic Chemistry</i> , 2018, 57, 12697-12708. | 1.9 | 16 |
| 11907 | Scalable and Highly Diastereo- and Enantioselective Catalytic Diels-Alder Reaction of $\hat{1},\hat{2}$ -Unsaturated Methyl Esters. <i>Journal of the American Chemical Society</i> , 2018, 140, 12671-12676. | 6.6 | 52 |
| 11908 | Unexpected formation of polymeric silver(I) complexes of azine-type ligand via self-assembly of Ag-salts with isatin oxamohydrazide. <i>Royal Society Open Science</i> , 2018, 5, 180434. | 1.1 | 7 |
| 11909 | Boron chelate complexes: X-ray and UV photoelectron spectra and electronic structure. <i>Russian Chemical Bulletin</i> , 2018, 67, 1153-1166. | 0.4 | 7 |
| 11910 | Accurate 13-C and 15-N molecular crystal chemical shielding tensors from fragment-based electronic structure theory. <i>Solid State Nuclear Magnetic Resonance</i> , 2018, 96, 10-18. | 1.5 | 17 |
| 11911 | Unraveling the Effects of H ₂ , N Substituents and Secondary Ligands on Cr/PNP-Catalyzed Ethylene Selective Oligomerization. <i>Organometallics</i> , 2018, 37, 3893-3900. | 1.1 | 16 |
| 11912 | Adsorption Mechanism of Molybdenum(VI) on Manganese Oxides Causing a Large Isotope Fractionation. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 1187-1195. | 1.2 | 13 |
| 11913 | Role of hydrogen bonding in the conformations of lidocaine, mepivacaine and bupivacaine under aqueous solvation. <i>Computational and Theoretical Chemistry</i> , 2018, 1144, 9-17. | 1.1 | 2 |
| 11914 | Electronic and Hydrogen Storage Properties of Li-Terminated Linear Boron Chains Studied by TAO-DFT. <i>Scientific Reports</i> , 2018, 8, 13538. | 1.6 | 32 |
| 11915 | Diffusion Monte Carlo calculations on LaB molecule. <i>Chinese Physics B</i> , 2018, 27, 093102. | 0.7 | 4 |
| 11916 | Mechanistic insight into the Rh-catalyzed mono- and double-decarbonylation of 1,4-diphenylbut-3-yne-1,2-dione: A computational study. <i>Journal of Organometallic Chemistry</i> , 2018, 877, 32-36. | 0.8 | 2 |
| 11917 | A Simple Correction for Nonadditive Dispersion within Extended Symmetry-Adapted Perturbation Theory (XSAPT). <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5128-5142. | 2.3 | 19 |
| 11918 | Synthesis of Expanded Porphyrinoids with Azulene and Indene Subunits and an opp-Dioxadibaporphyrin from Fulvene Carbinols and a Dioxacarbatrpyrrin. <i>Journal of Organic Chemistry</i> , 2018, 83, 12619-12631. | 1.7 | 23 |
| 11919 | Conformational Features of Thioamide-Containing Dipeptoids and Peptoid-Peptide Hybrids-Computational and Experimental Approaches. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7819-7831. | 1.1 | 2 |
| 11920 | Structure-Based Theory of Fluctuation-Induced Energy Transfer in a Molecular Dyad. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5940-5947. | 2.1 | 15 |
| 11921 | Organocatalytic [6+4] Cycloadditions via Zwitterionic Intermediates: Chemo-, Regio-, and Stereoselectivities. <i>Journal of the American Chemical Society</i> , 2018, 140, 13726-13735. | 6.6 | 37 |
| 11922 | Catalysis and tunnelling in the unimolecular decay of Criegee intermediates. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25224-25234. | 1.3 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 11923 | Instrumentation for Vibrational Circular Dichroism Spectroscopy: Method Comparison and Newer Developments. <i>Molecules</i> , 2018, 23, 2404. | 1.7 | 26 |
| 11924 | Rationally designing mixed Cu ^{1/4} -O ^{3/4} (M = Cu, Ag, Zn, Au) centers over zeolite materials with high catalytic activity towards methane activation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26522-26531. | 1.3 | 24 |
| 11925 | From Transition Metals to Lanthanides to Actinides: Metal-Mediated Tuning of Electronic Properties of Isostructural Metal-Organic Frameworks. <i>Inorganic Chemistry</i> , 2018, 57, 13246-13251. | 1.9 | 80 |
| 11926 | The Nonlocal Kernel in van der Waals Density Functionals as an Additive Correction: An Extensive Analysis with Special Emphasis on the B97M-V and P ⁰ B97M-V Approaches. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5725-5738. | 2.3 | 170 |
| 11927 | Trapping Iron(III)-Oxo Species at the Boundary of the α -Oxo Wall: Insights into the Nature of the Fe(III)-O Bond. <i>Journal of the American Chemical Society</i> , 2018, 140, 14391-14400. | 6.6 | 47 |
| 11928 | A combined experimental/theoretical approach to accelerated fuel cell development by quantitative prediction of redox potentials. <i>Journal of Power Sources</i> , 2018, 399, 443-447. | 4.0 | 2 |
| 11929 | Synthesis, characterization and biological evaluation of a nanorod five-coordinated Sn(IV) complex. Theoretical studies of (CH ₃) ₂ Sn(O) ₂ PPH ₂) ₂ . <i>Applied Organometallic Chemistry</i> , 2018, 32, e4610. | 1.7 | 6 |
| 11930 | Observation of the First Spin Crossover in an Iron(II) Complex with an S ₆ Coordination Environment: Tris[bis(<i>N</i>), <i>N</i>]-diethylamino)carbeniumdithiocarboxylato]iron(II) Hexafluorophosphate. <i>Chemistry - A European Journal</i> , 2018, 24, 17955-17963. | 1.7 | 6 |
| 11931 | Recent Developments in Density Functional Approximations. , 2018, , 1-14. | | 2 |
| 11932 | Influence of Charge Distribution on Structural Changes of Aromatic Imide Derivatives upon One-Electron Reduction Revealed by Time-Resolved Resonance Raman Spectroscopy during Pulse Radiolysis. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8738-8744. | 1.1 | 8 |
| 11933 | Explicit Method To Evaluate the External Reorganization Energy of Charge-Transfer Reactions in Oligoacene Crystals Using the State-Specific Polarizable Force Field. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8957-8964. | 1.1 | 10 |
| 11934 | Even-handed subsystem selection in projection-based embedding. <i>Journal of Chemical Physics</i> , 2018, 149, 144101. | 1.2 | 36 |
| 11935 | Verdazyls as Possible Building Blocks for Multifunctional Molecular Materials: A Case Study on 1,5-Diphenyl-3-(<i>p</i> -iodophenyl)-verdazyl Focusing on Magnetism, Electron Transfer and the Applicability of the Sonogashira-Hagihara Reaction. <i>Molecules</i> , 2018, 23, 1758. | 1.7 | 13 |
| 11936 | Fiber-Enhanced Raman Sensing of Cefuroxime in Human Urine. <i>Analytical Chemistry</i> , 2018, 90, 13243-13248. | 3.2 | 38 |
| 11937 | Properties of [Fe(Salten)Cl] Being a Precursor for Spin-Crossover Compounds in Polycrystals and Vitrified Acetonitrile Solutions. <i>Russian Journal of Inorganic Chemistry</i> , 2018, 63, 1012-1018. | 0.3 | 6 |
| 11938 | Si-atoms substitutions effects on the electronic and optical properties of coronene and ovalene. <i>New Journal of Physics</i> , 2018, 20, 113008. | 1.2 | 23 |
| 11939 | Quinolinol-based Al/Triarylborane Dyad Assembly: Alteration of Electronic Transition States Mediated by Fluoride Anion Binding. <i>Bulletin of the Korean Chemical Society</i> , 2018, 39, 1294-1301. | 1.0 | 3 |
| 11940 | Detection and identification of genetic material via single-molecule conductance. <i>Nature Nanotechnology</i> , 2018, 13, 1167-1173. | 15.6 | 59 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11941 | Implicit Solvation Using a Generalized Finite-Difference Approach in CRYSTAL: Implementation and Results for Molecules, Polymers, and Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5969-5983. | 2.3 | 8 |
| 11942 | Mechanism of Boron-Catalyzed N-Alkylation of Primary and Secondary Arylamines with Ketones Using Silanes under ω -Wet-Conditions. <i>Organometallics</i> , 2018, 37, 3698-3707. | 1.1 | 10 |
| 11943 | Ta ₂ ⁺ -mediated ammonia synthesis from N ₂ and H ₂ at ambient temperature. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 11680-11687. | 3.3 | 84 |
| 11944 | Theoretical Investigation on the Low-Lying States of LaP Molecule. <i>Chinese Physics Letters</i> , 2018, 35, 103101. | 1.3 | 5 |
| 11945 | Cyclopropenium Enhanced Thiourea Catalysis. <i>Journal of Organic Chemistry</i> , 2018, 83, 13973-13980. | 1.7 | 24 |
| 11946 | Dimerization of Polycyclic Aromatic Hydrocarbon Molecules and Radicals under Flame Conditions. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8701-8708. | 1.1 | 27 |
| 11947 | Density functional theory and ab initio studies on hyperfine coupling constants of phosphinyl radicals. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25779. | 1.0 | 9 |
| 11948 | Combined Molecular Dynamics and Coordinate Driving Method for Automatic Reaction Pathway Search of Reactions in Solution. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5787-5796. | 2.3 | 21 |
| 11949 | Exploring the Conversion of Macrocyclic 2,2-Biaryl Bis(thioureas) into Cyclic Monothioureas: An Experimental and Computational Investigation. <i>Journal of Organic Chemistry</i> , 2018, 83, 14022-14035. | 1.7 | 3 |
| 11950 | Efficient Hybrid Functional and Basis Set Functions for DFT Calculation of Refractive Indices and Abbe Numbers of Organic Compounds. <i>Chemistry Letters</i> , 2018, 47, 1494-1497. | 0.7 | 8 |
| 11951 | Tuning Environmentally Friendly Chelate-Based Ionic Liquids for Highly Efficient and Reversible SO ₂ Chemisorption. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 15292-15300. | 3.2 | 32 |
| 11952 | Accuracy of theoretical catalysis from a model of iron-catalyzed ammonia synthesis. <i>Communications Chemistry</i> , 2018, 1, . | 2.0 | 11 |
| 11953 | Exploring High-Symmetry Lanthanide-Functionalized Polyoxopalladates as Building Blocks for Quantum Computing. <i>Inorganics</i> , 2018, 6, 101. | 1.2 | 7 |
| 11954 | H ₄ octox: Versatile Bimodal Octadentate Acyclic Chelating Ligand for Medicinal Inorganic Chemistry. <i>Journal of the American Chemical Society</i> , 2018, 140, 15487-15500. | 6.6 | 32 |
| 11955 | Quantum Chemical Studies on the Corrosion Inhibition of Fe ₇₈ B ₁₃ Si ₉ glassy alloy in Na ₂ SO ₄ Solution of Some Thiosemicarbazone Derivatives. <i>International Journal of Electrochemical Science</i> , 2018, 13, 8241-8259. | 0.5 | 8 |
| 11956 | Quantifying Density Errors in DFT. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6385-6392. | 2.1 | 67 |
| 11957 | Stereoselectivity, Different Oxidation States, and Multiple Spin States in the Cyclopropanation of Olefins Catalyzed by Fe ⁰ -Porphyrin Complexes. <i>ACS Catalysis</i> , 2018, 8, 11140-11153. | 5.5 | 27 |
| 11958 | Quantum chemical study of formation of Cu ^{II} -YIII metallamacrocyclic complexes based on glycinehydroximate ligands. <i>Russian Chemical Bulletin</i> , 2018, 67, 1173-1181. | 0.4 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 11959 | Influence of complexing species on the extraction of trivalent actinides from lanthanides with CyMe4â€“BTBP: a theoretical study. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2018, 318, 1453-1463. | 0.7 | 11 |
| 11960 | Application of quantum mechanical simulations for studying the radiolytic stability of prospective extractants in the nuclear fuel cycle. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2018, 318, 2407-2413. | 0.7 | 7 |
| 11961 | Propylene Oxide Formation on a Silica Surface with Peroxo Defects: Implications in Astrochemistry. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9100-9106. | 1.1 | 7 |
| 11962 | Understanding the Influence of Surface Solvation and Structure on Polymorph Stability: A Combined Mechanochemical and Theoretical Approach. <i>Journal of the American Chemical Society</i> , 2018, 140, 17051-17059. | 6.6 | 51 |
| 11963 | Modeling the Oxygen Vacancy at a Molecular Vanadium(III) Silica-Supported Catalyst. <i>Journal of the American Chemical Society</i> , 2018, 140, 14903-14914. | 6.6 | 26 |
| 11964 | A computational study on molecular structure and stability of tautomers of dipyrrole-based phenanthroline analogue. <i>Computational and Theoretical Chemistry</i> , 2018, 1145, 6-14. | 1.1 | 3 |
| 11965 | Theoretical investigation of the structures, stabilities and vibrational properties of triatomic interhalide ions and their alkali ion pairs. <i>Journal of Fluorine Chemistry</i> , 2018, 216, 81-88. | 0.9 | 8 |
| 11966 | Decomposition of d- and f-Shell Contributions to Uranium Bonding from the Quantum Theory of Atoms in Molecules: Application to Uranium and Uranyl Halides. <i>Inorganics</i> , 2018, 6, 88. | 1.2 | 19 |
| 11967 | The Quantum Mechanics of a Rolling Molecular â€œNanocarâ€“. <i>Scientific Reports</i> , 2018, 8, 14878. | 1.6 | 3 |
| 11968 | Pyrolysis of the Cellulose Fraction of Biomass in the Presence of Solid Acid Catalysts: An Operando Spectroscopy and Theoretical Investigation. <i>ChemSusChem</i> , 2018, 11, 4044-4059. | 3.6 | 7 |
| 11969 | Calculating Optical Rotatory Dispersion Spectra in Solution Using a Smooth Dielectric Model. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8557-8564. | 1.1 | 6 |
| 11970 | Photoinduced O ₂ -Dependent Stepwise Oxidative Deglycation of a Nonheme Iron(III) Complex. <i>Journal of the American Chemical Society</i> , 2018, 140, 14150-14160. | 6.6 | 11 |
| 11971 | Structures, Spectroscopic Properties, and Dioxygen Reactivity of 5- and 6-Coordinate Nonheme Iron(II) Complexes: A Combined Enzyme/Model Study of Thiol Dioxygenases. <i>Journal of the American Chemical Society</i> , 2018, 140, 14807-14822. | 6.6 | 31 |
| 11972 | Phosphorescent Cyclometalated Platinum(II) aNHC Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 15603-15612. | 1.7 | 17 |
| 11973 | Dehydration Pathways for Glucose and Cellobiose During Fast Pyrolysis. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8071-8085. | 1.1 | 31 |
| 11974 | Solutionâ€“Processable, Solid State Donorâ€“Acceptor Materials for Singlet Fission. <i>Advanced Energy Materials</i> , 2018, 8, 1801720. | 10.2 | 21 |
| 11975 | Synthesis of 1,2-Diphospholides Using a Main Group â€œSuperbaseâ€“. <i>Organometallics</i> , 2018, 37, 4465-4472. | 1.1 | 4 |
| 11976 | Exciton localization in excited-state dynamics of a tetracene trimer: a surface hopping LC-TDDFTB study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25995-26007. | 1.3 | 23 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11977 | Computational Tools for Calculating log β^2 Values of Geochemically Relevant Uranium Organometallic Complexes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8007-8019. | 1.1 | 10 |
| 11978 | Rare and Nonexistent Nitrosyls: Periodic Trends and Relativistic Effects in Ruthenium and Osmium Porphyrin-Based $\{MNO\}^{7+}$ Complexes. <i>ACS Omega</i> , 2018, 3, 10513-10516. | 1.6 | 10 |
| 11979 | Enhanced quantum yields by sterically demanding aryl-substituted β^2 -diketonate ancillary ligands. <i>Beilstein Journal of Organic Chemistry</i> , 2018, 14, 664-671. | 1.3 | 17 |
| 11980 | Analysis of the variables that modify the robustness of Ti-SiO ₂ catalysts for alkene epoxidation: Role of silylation, deactivation and potential solutions. <i>Molecular Catalysis</i> , 2018, 459, 55-60. | 1.0 | 9 |
| 11981 | Combined Effects of Backbone and N-Substituents on Structure, Bonding, and Reactivity of Alkylated Iron(II)-NHCs. <i>Organometallics</i> , 2018, 37, 3093-3101. | 1.1 | 16 |
| 11982 | Metal- and Acid-Free C-H Formylation of Nitrogen Heterocycles: Using Trioxane as an Aldehyde Equivalent Enabled by an Organic-Soluble Oxidant. <i>Organic Letters</i> , 2018, 20, 5752-5756. | 2.4 | 24 |
| 11983 | The mechanism and origin of the regioselectivity of cobalt-catalyzed annulation of allenes with benzamide: a computational study. <i>Dalton Transactions</i> , 2018, 47, 13592-13601. | 1.6 | 2 |
| 11984 | Activating Aromatic Rings as Na-Ion Storage Sites to Achieve High Capacity. <i>CheM</i> , 2018, 4, 2463-2478. | 5.8 | 82 |
| 11985 | Pesticide byproducts formation: Theoretical study of the protonation of alloxidim degradation products. <i>Computational and Theoretical Chemistry</i> , 2018, 1143, 9-19. | 1.1 | 8 |
| 11986 | Structure and Magnetism of Seven-Coordinate Fe ^{III} , Fe ^{II} , Co ^{II} and Ni ^{II} Complexes Containing a Heptadentate 15-Membered Pyridine-Based Macrocyclic Ligand. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 4286-4297. | 1.0 | 26 |
| 11987 | Electronic Structure Origins of Surface-Dependent Growth in III-V Quantum Dots. <i>Chemistry of Materials</i> , 2018, 30, 7154-7165. | 3.2 | 25 |
| 11988 | The β^1 -H-C-Hg agostic interactions in the mercury complexes of N-confused porphyrin. <i>Dalton Transactions</i> , 2018, 47, 14774-14784. | 1.6 | 7 |
| 11989 | A highly flexible molecule: The peculiar case of ethynyl isothiocyanate HCCNCS. <i>Journal of Chemical Physics</i> , 2018, 149, 104304. | 1.2 | 12 |
| 11990 | New monofunctional platinum(II) and palladium(II) complexes: Studies of the nucleophilic substitution reactions, DNA/BSA interaction, and cytotoxic activity. <i>Journal of Inorganic Biochemistry</i> , 2018, 189, 91-102. | 1.5 | 46 |
| 11991 | Role of Photoisomerization on the Photodetachment of the Photoactive Yellow Protein Chromophore. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8222-8228. | 1.1 | 13 |
| 11992 | Tautomerism and antioxidant activity of some 4-acylpyrazolone-based Schiff bases: a theoretical study. <i>RSC Advances</i> , 2018, 8, 30842-30850. | 1.7 | 15 |
| 11993 | Effects of Ancillary Ligands on Redox and Chemical Properties of Ruthenium Coordinated Azoaromatic Pincer. <i>Inorganic Chemistry</i> , 2018, 57, 11995-12009. | 1.9 | 29 |
| 11994 | Photophysical Properties of Tetracationic Ruthenium Complexes and Their Ter-Ionic Assemblies with Chloride. <i>Inorganic Chemistry</i> , 2018, 57, 12232-12244. | 1.9 | 13 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 11995 | A systematic electronic structure study of the O–O bond dissociation energy of hydrogen peroxide and the electron affinity of the hydroxyl radical. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1. | 0.5 | 7 |
| 11996 | The structural and electronic properties of TiO ₂ polymorphs towards water splitting reaction. <i>Journal of Materials Science: Materials in Electronics</i> , 2018, 29, 18282-18289. | 1.1 | 1 |
| 11997 | C–H Activation of Methane by Nickel–Methoxide Complexes: A Density Functional Theory Study. <i>Organometallics</i> , 2018, 37, 3111-3121. | 1.1 | 12 |
| 11998 | Converting organosulfur compounds to inorganic polysulfides against resistant bacterial infections. <i>Nature Communications</i> , 2018, 9, 3713. | 5.8 | 141 |
| 11999 | Electronic Energies Are Not Enough: An Ion Mobility-Aided, Quantum Chemical Benchmark Analysis of H ₂ GPGG Conformers. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5406-5418. | 2.3 | 7 |
| 12000 | Quantum Tunneling Tautomer of <i>N,N</i> -Dimethyl- <i>p</i> -toluidine Dehydrogenates Identified by Deep-UV Laser Ionization Mass Spectroscopy. <i>ACS Omega</i> , 2018, 3, 10743-10747. | 1.6 | 2 |
| 12001 | Layer-Stacking-Driven Fluorescence in a Two-Dimensional Imine-Linked Covalent Organic Framework. <i>Journal of the American Chemical Society</i> , 2018, 140, 12922-12929. | 6.6 | 147 |
| 12002 | Wannier-Koopmans method calculations of organic molecule crystal band gaps. <i>Europhysics Letters</i> , 2018, 123, 37002. | 0.7 | 3 |
| 12003 | Understanding the role of ethylene glycol in a remarkable catalyst-free Strecker reaction of <i>α</i> -CF ₃ ketoimine: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2018, 1142, 57-65. | 1.1 | 0 |
| 12004 | Probing charge transfer characteristics in a donor–acceptor metal–organic framework by Raman spectroelectrochemistry and pressure-dependence studies. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25772-25779. | 1.3 | 28 |
| 12005 | New Tridentate Schiff Base, Product of Condensation of 4-Methyl-7-hydroxy-8-formylcoumarin and N-Aminomercaptotriazole: Synthesis, Structure, and Complex Formation. <i>Russian Journal of General Chemistry</i> , 2018, 88, 1441-1450. | 0.3 | 1 |
| 12007 | Theoretical and experimental evidence of conformational transformation in stereoisomers of nucleoside analogues. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25714. | 1.0 | 0 |
| 12008 | Effect of the Number and Substitution Pattern of Carbazole Donors on the Singlet and Triplet State Energies in a Series of Carbazole-Oxadiazole Derivatives Exhibiting Thermally Activated Delayed Fluorescence. <i>Chemistry of Materials</i> , 2018, 30, 6389-6399. | 3.2 | 17 |
| 12009 | A Strain-Deformation Nexus within Pincer Ligands: Application to the Spin States of Iron(II) Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 12312-12322. | 1.9 | 22 |
| 12010 | Relevance of Protons in Heterolytic Activation of H ₂ O ₂ over Nb(V): Insights from Model Studies on Nb-Substituted Polyoxometalates. <i>ACS Catalysis</i> , 2018, 8, 9722-9737. | 5.5 | 52 |
| 12011 | Supplementary data for the quantum chemical calculation of free radical substitution reaction mechanism of camptothecin. <i>Data in Brief</i> , 2018, 19, 2305-2310. | 0.5 | 0 |
| 12012 | Kinetic modeling for unimolecular β -scission of the methoxymethyl radical from quantum chemical and RRKM analyses. <i>Combustion and Flame</i> , 2018, 197, 243-253. | 2.8 | 8 |
| 12013 | Mechanistic insight into the ruthenium-catalyzed cycloaddition of enynes with alkynes: A theoretical study. <i>Journal of Organometallic Chemistry</i> , 2018, 875, 46-51. | 0.8 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12014 | Rotationally resolved electronic spectroscopy of 3-cyanoindole and the 3-cyanoindole-water complex. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 23441-23452. | 1.3 | 15 |
| 12015 | Anion coordination directed synthesis patterns for [Ni ₄] aggregates: structural changes for thiocyanate coordination and ligand arm hydrolysis. <i>New Journal of Chemistry</i> , 2018, 42, 16717-16728. | 1.4 | 14 |
| 12016 | Prediction of ¹ H NMR chemical shifts for ionic liquids: strategy and application of a relative reference standard. <i>RSC Advances</i> , 2018, 8, 28604-28612. | 1.7 | 12 |
| 12017 | Novel self-adaptive boat-shaped complexes with a tetrakisphosphine ligand. <i>Dalton Transactions</i> , 2018, 47, 13689-13695. | 1.6 | 1 |
| 12018 | A turn-on fluorescent probe based on Si-rhodamine for sensitive and selective detection of phosgene in solution and in the gas phase. <i>Journal of Materials Chemistry C</i> , 2018, 6, 10472-10479. | 2.7 | 54 |
| 12019 | Theoretical Study of C ₂ H ₅ + NCO Reaction: Mechanism and Kinetics. <i>Journal of Chemistry</i> , 2018, 2018, 1-8. | 0.9 | 1 |
| 12020 | In Situ Doping Boron Atoms into Porous Carbon Nanoparticles with Increased Oxygen Graft Enhances both Affinity and Durability toward Electrolyte for Greatly Improved Supercapacitive Performance. <i>Advanced Functional Materials</i> , 2018, 28, 1804190. | 7.8 | 149 |
| 12021 | Planar ten-membered 10- π -electron aromatic (CH) ₅ (XH) ₅ {X = Ge, Sn} systems. <i>Journal of Molecular Modeling</i> , 2018, 24, 264. | 0.8 | 0 |
| 12022 | Diheme Cytochrome <i>c</i> : Structure-Function Correlation and Effect of Heme-Heme Interactions. <i>Inorganic Chemistry</i> , 2018, 57, 11498-11510. | 1.9 | 23 |
| 12023 | Naphtho[2,3- <i>b</i>]carbaporphyrins. <i>Journal of Organic Chemistry</i> , 2018, 83, 11825-11838. | 1.7 | 18 |
| 12024 | Time-Dependent Density-Functional Theory for Modeling Solid-State Fluorescence Emission of Organic Multicomponent Crystals. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7514-7521. | 1.1 | 9 |
| 12025 | Highly Specific Enrichment of Multi-phosphopeptides by the Diphosphorylated Fructose-Modified Dual-Metal-Centered Zirconium-Organic Framework. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 32613-32621. | 4.0 | 38 |
| 12026 | Computational Mechanistic Analysis of Intramolecular Cycloadditions of the 1,3-Dithiolium Cation with Adjacent Alkene and Allene Functional Groups. <i>ACS Omega</i> , 2018, 3, 9770-9780. | 1.6 | 4 |
| 12027 | From interstellar carbon monosulfide to methyl mercaptan: paths of least resistance. <i>Astronomy and Astrophysics</i> , 2018, 615, L2. | 2.1 | 23 |
| 12028 | Fitting a round peg into a round hole: Asymptotically correcting the generalized gradient approximation for correlation. <i>Journal of Chemical Physics</i> , 2018, 149, 084116. | 1.2 | 33 |
| 12029 | Communication: Optical gap in polyacetylene from a simple quantum chemistry exciton model. <i>Journal of Chemical Physics</i> , 2018, 149, 081102. | 1.2 | 11 |
| 12030 | First-Principles Studies of the Magnetic Structure and Exchange Interactions of β -EtnMe ₄ nZ[Pd(dmit) ₂]. <i>Journal of the Physical Society of Japan</i> , 2018, 87, 124709. | 0.7 | 0 |
| 12031 | Sulfides and Disulfides of s-Triazine: Potential Thermal Thiyl Radical Generators. <i>Chemistry - A European Journal</i> , 2018, 24, 13596-13606. | 1.7 | 11 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12032 | Structures and bonding properties of Pd n C 2 $\hat{\alpha}^{\prime\prime}/0$ ($\hat{n}\hat{\epsilon}^{\prime}=\hat{\alpha}\hat{\epsilon}^{\prime}1\hat{\alpha}\hat{\epsilon}^{\prime\prime}7$) clusters. <i>Chemical Physics Letters</i> , 2018, 705, 65-70. | 1.2 | 1 |
| 12033 | Systematic design of indium-based luminophores with color-tunable emission via combined manipulation of HOMO and LUMO levels. <i>Dyes and Pigments</i> , 2018, 158, 285-294. | 2.0 | 17 |
| 12034 | Synthesis, spectral characterization, reactivity and DFT studies of novel ligand phenylseleno benzylacetate (L) and its complexes with group 12 metal chlorides. <i>Journal of Molecular Structure</i> , 2018, 1171, 233-242. | 1.8 | 16 |
| 12035 | Mechanism of Photocatalytic Cyclization of Bromoalkenes with a Dimeric Gold Complex. <i>Organometallics</i> , 2018, 37, 1725-1733. | 1.1 | 9 |
| 12036 | Cluster-model DFT simulations of the infrared spectra of triazine-based molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 20779-20784. | 1.3 | 14 |
| 12037 | Unimolecular reaction of acetone oxide and its reaction with water in the atmosphere. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 6135-6140. | 3.3 | 76 |
| 12038 | Alkyl Radical Generation by an Intramolecular Homolytic Substitution Reaction between Iron(II) and Trialkylsulfonium Groups. <i>Chemistry - A European Journal</i> , 2018, 24, 11008-11020. | 1.7 | 6 |
| 12039 | Generation of methylene by the liquid phase oxidation of isobutene with nitrous oxide. <i>Tetrahedron</i> , 2018, 74, 3589-3595. | 1.0 | 6 |
| 12040 | QM/MM simulations identify the determinants of catalytic activity differences between type II dehydroquinase enzymes. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 4443-4455. | 1.5 | 19 |
| 12041 | Theoretical and experimental investigations into structural, electronic, molecular and biological properties of 4-(3-chlorophenyl)-1-(3-chloropropyl) piperazin-1-ium chloride. <i>Journal of Molecular Structure</i> , 2018, 1168, 242-249. | 1.8 | 19 |
| 12042 | Torsional Bias as a Strategy To Tune Singlet-Triplet Gaps in Organic Diradicals. <i>Journal of Physical Chemistry C</i> , 2018, 122, 12148-12157. | 1.5 | 7 |
| 12043 | The serendipitous discovery of a readily available redox-bistable molecule derived from cyclic(alkyl)(amino)carbenes. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2073-2078. | 2.3 | 10 |
| 12044 | Mechanistic Insights into Selective Oxidation of Polyaromatic Compounds using RICO Chemistry. <i>Chemistry - A European Journal</i> , 2018, 24, 12359-12369. | 1.7 | 7 |
| 12045 | Exploring conformational preferences of alanine tetrapeptide by CCSD(T), MP2, and dispersion-corrected DFT methods. <i>Chemical Physics Letters</i> , 2018, 702, 69-75. | 1.2 | 12 |
| 12046 | A combined time-resolved infrared and density functional theory study of the lowest excited states of 9-fluorenone and 2-naphthaldehyde. <i>Chemical Physics</i> , 2018, 512, 44-52. | 0.9 | 9 |
| 12047 | A Tricopper(I) Complex Competent for O Atom Transfer, C-H Bond Activation, and Multiple O ₂ Activation Steps. <i>Inorganic Chemistry</i> , 2018, 57, 11361-11368. | 1.9 | 14 |
| 12048 | Pyridyl group design in viologens for anolyte materials in organic redox flow batteries. <i>RSC Advances</i> , 2018, 8, 18762-18770. | 1.7 | 23 |
| 12049 | A photoelectron imaging and quantum chemistry study of the deprotonated indole anion. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 15543-15549. | 1.3 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 12050 | Zwitterions of the excited 4-([2,2'-bipyridine]-4-yl) phenol photoacid molecules: Formation and fluorescence. <i>Journal of Molecular Liquids</i> , 2018, 264, 48-53. | 2.3 | 24 |
| 12051 | Controlling the Reaction Steps of Bifunctional Molecules 1,5-Dibromo-2,6-dimethylnaphthalene on Different Substrates. <i>Journal of Physical Chemistry C</i> , 2018, 122, 13001-13008. | 1.5 | 21 |
| 12052 | Extent of Fock-exchange mixing for a hybrid van der Waals density functional?. <i>Journal of Chemical Physics</i> , 2018, 148, 194115. | 1.2 | 17 |
| 12053 | Protein-Assisted Formation and Stabilization of Catalytically Active Polyoxometalate Species. <i>Chemistry - A European Journal</i> , 2018, 24, 10099-10108. | 1.7 | 45 |
| 12054 | Substituent effects on the oxidation reactions of 4-nitrophenol, phenol, 4-methylphenol, and 4-methoxyphenol mediated by reduced graphene oxide in water. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2018, 553, 35-41. | 2.3 | 2 |
| 12055 | Mechanistic investigations of Co(II)-Catalyzed C-N coupling reactions. <i>Journal of Organometallic Chemistry</i> , 2018, 868, 144-153. | 0.8 | 16 |
| 12056 | Cold physics and chemistry: Collisions, ionization and reactions inside helium nanodroplets close to zero K. <i>Physics Reports</i> , 2018, 751, 1-90. | 10.3 | 113 |
| 12057 | Substituted 1-(isoxazol-3-yl)methyl-1H-1,2,3-triazoles: Synthesis, palladium(II) complexes, and high-turnover catalysis in aqueous media. <i>Tetrahedron</i> , 2018, 74, 3578-3588. | 1.0 | 10 |
| 12058 | Redox-triggered chiroptical switching activity of ruthenium(III)-bis(1,2-diketonato) complexes bearing a bipyridine-helicene ligand. <i>Chirality</i> , 2018, 30, 592-601. | 1.3 | 12 |
| 12059 | Chemical Bond Energies of 3d Transition Metals Studied by Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3479-3492. | 2.3 | 64 |
| 12060 | Structural Diversity in a New Series of Halogenated Quinoly Salicylaldimides-Based Fe ^{III} Complexes Showing Solid-State Halogen-Bonding/Halogen-Halogen Interactions. <i>Crystal Growth and Design</i> , 2018, 18, 4187-4199. | 1.4 | 10 |
| 12061 | Electronic structure and photoabsorption of Ti ³⁺ ions in reduced anatase and rutile TiO ₂ . <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17658-17665. | 1.3 | 38 |
| 12062 | Turning on Solid-State Fluorescence with Light. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 9538-9542. | 7.2 | 6 |
| 12063 | Structural Assignment of Fluorocyclobutenes by ¹⁹ F NMR Spectroscopy – Comparison of Calculated ¹⁹ F NMR Shielding Constants with Experimental ¹⁹ F NMR Shifts. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 3867-3874. | 1.2 | 5 |
| 12064 | Correlations between the ¹ H NMR chemical shieldings and the pK _a values of organic acids and amines. <i>Journal of Molecular Modeling</i> , 2018, 24, 146. | 0.8 | 3 |
| 12065 | Radical Rearrangement Chemistry in Ultraviolet Photodissociation of Iodotyrosine Systems: Insights from Metastable Dissociation, Infrared Ion Spectroscopy, and Reaction Pathway Calculations. <i>Journal of the American Society for Mass Spectrometry</i> , 2018, 29, 1791-1801. | 1.2 | 10 |
| 12066 | Femtosecond Fluorescence Upconversion Study of a Naphthalimide-Bithiophene-Triphenylamine Push-Pull Dye in Solution. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5533-5544. | 1.1 | 13 |
| 12067 | Possibility of Protic Ionic Liquids Formation From Triethanolamine with Sulfonamides. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6586-6594. | 1.2 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12068 | Influence of electron donors in fluorescent NLOphoric D- π -A derivatives with acenaphthene rotor: Photophysical, viscosity, and TD-DFT studies. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 364, 40-52. | 2.0 | 5 |
| 12069 | A New Candidate Laser Dye Based 1,4-Bis[π^2 -(2-Naphthothiazolyle)Vinyl]Benzene. Spectroscopic Behavior, Laser Parameters and Excitation Energy Transfer. <i>Journal of Fluorescence</i> , 2018, 28, 743-758. | 1.3 | 5 |
| 12070 | Anhydrous proline crystals: Structural optimization, optoelectronic properties, effective masses and Frenkel exciton energy. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 121, 36-48. | 1.9 | 17 |
| 12071 | Strict Correlation of HOMO Topology and Magnetic Aromaticity Indices in d-Block Metalloaromatics. <i>Chemistry - A European Journal</i> , 2018, 24, 10059-10063. | 1.7 | 15 |
| 12072 | IR, Raman, and Vibrational Optical Activity Spectra of Methyl Glycidate in Chloroform and Water: The <i>Clusters in a Liquid</i> Solvation Model. <i>ChemPhysChem</i> , 2018, 19, 2234-2242. | 1.0 | 21 |
| 12073 | Benchmarking DFT methods on linear and nonlinear electric properties of spatially confined molecules. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25666. | 1.0 | 14 |
| 12074 | The role of sulfate in the chemical synthesis of graphene oxide. <i>Materials Chemistry and Physics</i> , 2018, 215, 203-210. | 2.0 | 12 |
| 12075 | Assessment of Density Functional Methods for Geometry Optimization of Bimolecular van der Waals Complexes. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3004-3013. | 2.3 | 27 |
| 12076 | Density Functional Theory for Microwave Spectroscopy of Noncovalent Complexes: A Benchmark Study. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4894-4901. | 1.1 | 20 |
| 12077 | Vibrational spectra of alkylamino substituted phthalocyanine compounds: Density functional theory calculations. <i>Journal of Porphyrins and Phthalocyanines</i> , 2018, 22, 771-776. | 0.4 | 4 |
| 12078 | Does the Intramolecular Hydrogen Bond Affect the Spectroscopic Properties of Bicyclic Diazole Heterocycles?. <i>Journal of Spectroscopy</i> , 2018, 2018, 1-15. | 0.6 | 5 |
| 12079 | Palladium-Catalyzed Aerobic Homocoupling of Alkynes: Full Mechanistic Characterization of a More Complex Oxidase-Type Behavior. <i>ACS Catalysis</i> , 2018, 8, 7495-7506. | 5.5 | 30 |
| 12080 | A Theoretical Investigation of the Reaction H+SiS ₂ and Implications for the Chemistry of Silicon in the Interstellar Medium. <i>Lecture Notes in Computer Science</i> , 2018, , 719-729. | 1.0 | 2 |
| 12081 | A Theoretical Investigation of the Reaction N(2D) \hat{A} +C ₆ H ₆ and Implications for the Upper Atmosphere of Titan. <i>Lecture Notes in Computer Science</i> , 2018, , 763-772. | 1.0 | 10 |
| 12083 | Computational study of energy materials. , 2018, , 263-281. | | 0 |
| 12084 | When Hartree-Fock exchange admixture lowers DFT-predicted barrier heights: Natural bond orbital analyses and implications for catalysis. <i>Journal of Chemical Physics</i> , 2018, 148, 244106. | 1.2 | 25 |
| 12085 | Static correlated functionals for reduced density matrix functional theory. <i>European Physical Journal B</i> , 2018, 91, 1. | 0.6 | 10 |
| 12086 | Design, synthesis, DFT, docking studies and ADME prediction of some new coumarinyl linked pyrazolylthiazoles: Potential standalone or adjuvant antimicrobial agents. <i>PLoS ONE</i> , 2018, 13, e0196016. | 1.1 | 71 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12087 | High-Throughput Screening Approach for the Optoelectronic Properties of Conjugated Polymers. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 2450-2459. | 2.5 | 57 |
| 12088 | Gas sensing behavior of metal-phthalocyanines: Effects of electronic structure on sensitivity. <i>Chemical Physics</i> , 2018, 513, 23-34. | 0.9 | 31 |
| 12089 | Helicity and Topological Chirality in Hydrogen-Bonded Supermolecules Characterized by Advanced Graph Set Analysis and Solid-State Vibrational Circular Dichroism Spectroscopy. <i>Crystal Growth and Design</i> , 2018, 18, 4621-4627. | 1.4 | 15 |
| 12090 | Absorption Spectroscopy and Photophysics of a Re^{I} - dppz Probe for DNA-Mediated Charge Transport. <i>Chemistry - A European Journal</i> , 2018, 24, 14425-14435. | 1.7 | 9 |
| 12091 | Solvent Control of Ligand-Metal Electron Transfer in Mononuclear Copper Complexes with Redox-Active Bisguanidine Ligands. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 3660-3667. | 1.0 | 16 |
| 12092 | Synthesis, characterization, and crystal structure of novel bulky phenyl-bridged Ti^{II} -diimine binucleating ligands. <i>Heteroatom Chemistry</i> , 2018, 29, . | 0.4 | 0 |
| 12093 | New High Pressure Phases of Energetic Material TEX: Evidence from Raman Spectroscopy, X-ray Diffraction, and First-Principles Calculations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6236-6242. | 1.1 | 13 |
| 12094 | Inclusions of Si-atoms in Graphene nanostructures: a computational study on the ground-state electronic properties of Coronene and Ovalene. <i>Journal of Physics: Conference Series</i> , 2018, 956, 012020. | 0.3 | 16 |
| 12095 | Anschalten von Festkörperlumineszenz mit Licht. <i>Angewandte Chemie</i> , 2018, 130, 9683-9687. | 1.6 | 1 |
| 12096 | Magnetic Anisotropy, Magneto-Structural Correlations and Mechanism of Magnetic Relaxation in $\{\text{Dy}^{\text{III}}\text{N}_8\}$ Complexes: A Theoretical Perspective. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 3402-3412. | 1.0 | 12 |
| 12097 | Low-Spin Fe(III) Macrocyclic Complexes of Imidazole-Appended 1,4,7-Triazacyclononane as Paramagnetic Probes. <i>Inorganic Chemistry</i> , 2018, 57, 8364-8374. | 1.9 | 34 |
| 12098 | Isotope Effects Reveal an Alternative Mechanism for α -Aluminium-Ion-Catalysis. <i>Journal of the American Chemical Society</i> , 2018, 140, 8396-8400. | 6.6 | 13 |
| 12099 | Molecular dynamics and quantum chemistry-based approaches to identify isoform selective HDAC2 inhibitor "a novel target to prevent Alzheimer's disease. <i>Journal of Receptor and Signal Transduction Research</i> , 2018, 38, 266-278. | 1.3 | 13 |
| 12100 | Formation of Nitrogen-Bearing Organic Molecules in the Reaction $\text{NH}_3 + \text{C}_2\text{H}_5$: A Theoretical Investigation and Main Implications for Prebiotic Chemistry in Space. <i>Lecture Notes in Computer Science</i> , 2018, , 773-782. | 1.0 | 3 |
| 12101 | Improvement of multiferroic property and change of magnetic ordering in new ANiO_3 ($\text{A} = \text{Ti, Ge, Zr, Sn}$). <i>Tj ETQq0 0 0 rgt /Overlo</i> | 1.4 | 13 |
| 12102 | Computational screening and molecular design of anthracene-based semiconductors. <i>Organic Electronics</i> , 2018, 61, 87-95. | 1.4 | 5 |
| 12103 | A Series of 4- and 5-Coordinate Ni(II) Complexes: Synthesis, Characterization, Spectroscopic, and DFT Studies. <i>Inorganic Chemistry</i> , 2018, 57, 8307-8316. | 1.9 | 24 |
| 12104 | Spin Signature of the C_{60} Fullerene Anion: A Combined X- and D-Band EPR and DFT Study. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3915-3921. | 2.1 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 12105 | Curved TiO ₂ Nanoparticles in Water: Short (Chemical) and Long (Physical) Range Interfacial Effects. ACS Applied Materials & Interfaces, 2018, 10, 29943-29953. | 4.0 | 35 |
| 12106 | Structural evolution and bonding properties of Au ₂ Si ⁿ⁺ /O (n = 1-7) clusters: Anion photoelectron spectroscopy and theoretical calculations. Journal of Chemical Physics, 2018, 148, 244306. | 1.2 | 33 |
| 12107 | Identifying the Rate-Limiting Elementary Steps of Nitrogen Fixation with Single-Site Fe Model Complexes. Inorganic Chemistry, 2018, 57, 8499-8508. | 1.9 | 19 |
| 12108 | Performance of Property-Optimized Basis Sets for Optical Rotation with Coupled Cluster Theory. Journal of Physical Chemistry A, 2018, 122, 5962-5969. | 1.1 | 15 |
| 12109 | Defining the conditional basis of silicon phthalocyanine near-IR ligand exchange. Physical Chemistry Chemical Physics, 2018, 20, 19030-19036. | 1.3 | 18 |
| 12110 | Study on bridging moiety effect on asymmetric double D-π-A dyes. Organic Electronics, 2018, 62, 598-609. | 1.4 | 13 |
| 12111 | Exploiting Coordinate Scaling Relations To Accelerate Exact Exchange Calculations. Journal of Physical Chemistry Letters, 2018, 9, 3886-3890. | 2.1 | 8 |
| 12112 | New insights into the sensing mechanism of a phosphonate pyrene chemosensor for TNT. Physical Chemistry Chemical Physics, 2018, 20, 19539-19545. | 1.3 | 20 |
| 12113 | Experimental and theoretical study of aluminium corrosion in NaOH, NaCl and HCl solutions. Anti-Corrosion Methods and Materials, 2018, 65, 350-360. | 0.6 | 5 |
| 12114 | Can Path Integral Molecular Dynamics Make a Good Approximation for Vapor Pressure Isotope Effects Prediction for Organic Solvents? A Comparison to ONIOM QM/MM and QM Cluster Calculation. Journal of Physical Chemistry B, 2018, 122, 7353-7364. | 1.2 | 4 |
| 12115 | Anion photoelectron spectroscopy and chemical bonding of ThO ₂ ⁺ and ThO ₃ ⁺ . Journal of Chemical Physics, 2018, 148, 244304. | 1.2 | 6 |
| 12116 | Quantum-Chemical Study of Reaction Laws of 2,4,6-Triphenylpyranyl Radical with Oxygen. Russian Journal of Organic Chemistry, 2018, 54, 719-725. | 0.3 | 2 |
| 12117 | Meta-Selective C-H Alkylation of 2-Phenylpyridine Catalyzed by Ruthenium: DFT Study on the Mechanism and Regioselectivity. European Journal of Organic Chemistry, 2018, 2018, 5268-5277. | 1.2 | 16 |
| 12118 | Multi-redox Molecule for High-Energy Redox Flow Batteries. Joule, 2018, 2, 1771-1782. | 11.7 | 123 |
| 12119 | Synthesis and electronic structure studies of a novel nonlinear optical crystal L-leucinium squarate monohydrate: A spectroscopic view. Journal of Physics and Chemistry of Solids, 2018, 122, 143-153. | 1.9 | 11 |
| 12120 | Total Stereoselective Michael Addition of N- and S- Nucleophiles to a d-Erythrosyl 1,5-Lactone Derivative. Experimental and Theoretical Studies Devoted to the Synthesis of 2,6-Dideoxy-4-functionalized-ribo-1,4-lactone. Journal of Organic Chemistry, 2018, 83, 8011-8019. | 1.7 | 3 |
| 12121 | Reactivity of Tuck-over Titanium Oxo Complexes with Isocyanides. Organometallics, 2018, 37, 2046-2053. | 1.1 | 7 |
| 12122 | Intramolecular metal-ligand electron transfer triggered by co-ligand substitution. Dalton Transactions, 2018, 47, 9430-9441. | 1.6 | 18 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12123 | Frozen-density embedding as a quasi-diabatization tool: Charge-localized states for spin-density calculations. <i>Journal of Chemical Physics</i> , 2018, 148, 214104. | 1.2 | 13 |
| 12124 | Cytotoxic phloroglucinol meroterpenoid from <i>Eugenia umbelliflora</i> fruits. <i>Phytochemistry Letters</i> , 2018, 27, 187-192. | 0.6 | 17 |
| 12125 | Chromogenic, Fluorescent, and Redox Sensors for Multichannel Imaging and Detection of Hydrogen Peroxide in Living Cell Systems. <i>Analytical Chemistry</i> , 2018, 90, 10152-10158. | 3.2 | 59 |
| 12126 | Method Calibration or Data Fitting?. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4651-4661. | 2.3 | 27 |
| 12127 | Enhanced Stability of the Carba-closo-dodecaborate Anion for High-Voltage Battery Electrolytes through Rational Design. <i>Journal of the American Chemical Society</i> , 2018, 140, 11076-11084. | 6.6 | 80 |
| 12128 | Effective modulation of intramolecular ferromagnetic interaction of diradicals by functionalization of cross-conjugated coupler. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 20688-20694. | 1.3 | 6 |
| 12129 | Porphyrin-like Fe-N ₄ sites with sulfur adjustment on hierarchical porous carbon for different rate-determining steps in oxygen reduction reaction. <i>Nano Research</i> , 2018, 11, 6260-6269. | 5.8 | 118 |
| 12130 | Ultrafast Deep-Ultraviolet Laser Ionization Mass Spectrometry Applicable To Identify Phenylenediamine Isomers. <i>Analytical Chemistry</i> , 2018, 90, 10635-10640. | 3.2 | 19 |
| 12131 | Force Field Benchmark of Amino Acids. 2. Partition Coefficients between Water and Organic Solvents. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1669-1681. | 2.5 | 33 |
| 12132 | A chiral spiroborate anion from diphenyl-tartramide [B{Tar(NHPh) ₂ }] ⁺ applied to some challenging resolutions. <i>CrystEngComm</i> , 2018, 20, 4831-4848. | 1.3 | 5 |
| 12133 | CBS extrapolation in electronic structure pushed to the end: a revival of minimal and sub-minimal basis sets. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22084-22098. | 1.3 | 25 |
| 12134 | Novel-Substituted Heterocyclic GABA Analogues. Enzymatic Activity against the GABA-AT Enzyme from <i>Pseudomonas fluorescens</i> and In Silico Molecular Modeling. <i>Molecules</i> , 2018, 23, 1128. | 1.7 | 6 |
| 12135 | Structural, vibrational and thermal studies on bis(l-glutamato)copper(II). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 205, 603-613. | 2.0 | 10 |
| 12136 | Synthesis, structures, and reactivity studies of cyclometalated N-heterocyclic carbene complexes of ruthenium. <i>Dalton Transactions</i> , 2018, 47, 12138-12146. | 1.6 | 11 |
| 12137 | Effects of Thiolate Ligation in Monoiron Hydrogenase (Hmd): Stability of the {Fe(CO) ₂ } ²⁺ Core with NNS Ligands. <i>Inorganic Chemistry</i> , 2018, 57, 10028-10039. | 1.9 | 6 |
| 12138 | Matrix-isolation vibrational circular dichroism spectroscopy in structural studies of peptides: Conformational landscape of the Ac(-Ala)1-4-OMe depsipeptide series. <i>Journal of Molecular Spectroscopy</i> , 2018, 351, 29-38. | 0.4 | 6 |
| 12139 | DFT studies of isomerization in palladium(IV) chemistry and alkyl halide transfer from palladium(IV) to palladium(II). <i>Journal of Organometallic Chemistry</i> , 2018, 872, 110-113. | 0.8 | 1 |
| 12140 | Quantification of Aromaticity of Heterocyclic Systems Using Interaction Coordinates. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6953-6960. | 1.1 | 22 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 12141 | Single-Stranded DNA Oligonucleotides Retain Rise Coordinates Characteristic of Double Helices. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7978-7989. | 1.2 | 12 |
| 12142 | Conformational dynamics of 1-phenyl-2,2,2-trifluoroethanol by rotational spectroscopy and ab initio calculations. <i>Journal of Molecular Spectroscopy</i> , 2018, 351, 62-67. | 0.4 | 31 |
| 12143 | Silver-Stabilized Guanine Duplex: Structural and Optical Properties. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4789-4794. | 2.1 | 15 |
| 12144 | Dynamic kinetic resolution of 1-substituted-3-methyl-3-phospholene oxides via the formation of diastereomeric alkoxyphospholenium salts. <i>Tetrahedron</i> , 2018, 74, 5850-5857. | 1.0 | 5 |
| 12145 | Thermal azide-alkene cycloaddition reactions: straightforward multi-gram access to β -1,2,3-triazolines in deep eutectic solvents. <i>Green Chemistry</i> , 2018, 20, 4023-4035. | 4.6 | 30 |
| 12146 | cPCET versus HAT: A Direct Theoretical Method for Distinguishing X-H Bond-Activation Mechanisms. <i>Angewandte Chemie</i> , 2018, 130, 12089-12093. | 1.6 | 20 |
| 12147 | Stereodivergent Rhodium(III)-Catalyzed cis-Cyclopropanation Enabled by Multivariate Optimization. <i>Journal of the American Chemical Society</i> , 2018, 140, 9587-9593. | 6.6 | 55 |
| 12148 | Semi-empirical or non-empirical double-hybrid density functionals: which are more robust?. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 23175-23194. | 1.3 | 102 |
| 12149 | Aromaticity of some carbenes and their heavier analogs in light of gauge-including magnetically induced current approach as a new magnetic criterium. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25759. | 1.0 | 5 |
| 12150 | (10.4) Face of Ordered and Disordered Dolomite, MgCa(CO ₃) ₂ : A Computational Study to Reveal the Growth Mechanism. <i>Minerals (Basel, Switzerland)</i> , 2018, 8, 323. | 0.8 | 7 |
| 12151 | The Mechanism of Cyclodehydrofluorination on γ -Alumina. <i>Physica Status Solidi (B): Basic Research</i> , 2018, 255, 1800189. | 0.7 | 12 |
| 12152 | Structure, Bonding, Reactivity and Spectral Features of Putative Ni ^{III} =O Species: A Theoretical Perspective. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2018, 644, 790-800. | 0.6 | 3 |
| 12153 | Widely used hardly known. An insight into electric and dynamic properties of formamidinium iodide. <i>RSC Advances</i> , 2018, 8, 26506-26516. | 1.7 | 9 |
| 12154 | Redox-Active Chiroptical Switching in Mono- and Bis-iron Ethynylcarbo[6]helicenes Studied by Electronic and Vibrational Circular Dichroism and Resonance Raman Optical Activity. <i>Chemistry - A European Journal</i> , 2018, 24, 15067-15079. | 1.7 | 24 |
| 12155 | Mechanisms of the synthesis of trialkylsubstituted alkenylboronates from unactivated internal alkynes catalyzed by copper: A theoretical study. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 154-159. | 0.8 | 10 |
| 12156 | Combining Wave Function Methods with Density Functional Theory for Excited States. <i>Chemical Reviews</i> , 2018, 118, 7249-7292. | 23.0 | 166 |
| 12157 | Transferability in Machine Learning for Electronic Structure via the Molecular Orbital Basis. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4772-4779. | 2.3 | 149 |
| 12158 | Unraveling substituent effects on the glass transition temperatures of biorenewable polyesters. <i>Nature Communications</i> , 2018, 9, 2880. | 5.8 | 58 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12159 | Can Popular DFT Approximations and Truncated Coupled Cluster Theory Describe the Potential Energy Surface of the Beryllium Dimer?. Australian Journal of Chemistry, 2018, 71, 804. | 0.5 | 6 |
| 12160 | Copper(II) diclofenac complexes: Synthesis, structural studies and interaction with albumins and calf-thymus DNA. Journal of Inorganic Biochemistry, 2018, 187, 97-108. | 1.5 | 26 |
| 12161 | Chemical order in Ga or Sb modified germanium sulfide glasses around stoichiometry: High-resolution XPS and Raman studies. Journal of Non-Crystalline Solids, 2018, 499, 237-244. | 1.5 | 14 |
| 12162 | SERS and DFT study of indigo adsorbed on silver nanostructured surface. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 205, 465-469. | 2.0 | 24 |
| 12163 | The Dual Role of Gold(I) Complexes in Photosensitizer-Free Visible-Light-Mediated Gold-Catalyzed 1,2-Difunctionalization of Alkynes: A DFT Study. Chemistry - A European Journal, 2018, 24, 14119-14126. | 1.7 | 29 |
| 12164 | Examining the reaction between antioxidant compounds and 2,2-diphenyl-1-picrylhydrazyl (DPPH) through a computational investigation. Journal of Molecular Modeling, 2018, 24, 218. | 0.8 | 30 |
| 12165 | Communication: Correct charge transfer in CT complexes from the Becke's M05 density functional. Journal of Chemical Physics, 2018, 148, 211101. | 1.2 | 20 |
| 12166 | Coordination Compounds of Bivalent Metals with (Z)-4-(2-Hydroxy-5-nitrophenyl)hydrazono-3-methyl-1-phenyl-1H-pyrazol-5(4H)-one: Crystal and Molecular Structure of C ₁₆ H ₁₃ N ₅ O ₄ . Russian Journal of Inorganic Chemistry, 2018, 63, 874-880. | 0.3 | 2 |
| 12167 | Effects of Empirical Dispersion Energy on the Geometrical Parameters and Relative Energy of a Salicylideneaniline Molecular Switch in the Solid State. Crystals, 2018, 8, 125. | 1.0 | 6 |
| 12168 | Synthesis and Reactivity of Low-Valent f-Element Iodide Complexes with Neutral Iminophosphorane Ligands. Inorganic Chemistry, 2018, 57, 9230-9240. | 1.9 | 22 |
| 12169 | Graphene Oxide Quantum Dots as the Support for the Synthesis of Gold Nanoparticles and Their Applications as New Catalysts for the Decomposition of Composite Solid Propellants. ACS Omega, 2018, 3, 7278-7287. | 1.6 | 38 |
| 12170 | Electroanalytical detection of heavy metals using metallophthalocyanine and silica-coated iron oxide composites. Chemical Papers, 2018, 72, 3043-3056. | 1.0 | 15 |
| 12171 | Assessment of Ab Initio and Density Functional Theory Methods for the Excitations of Donor-Acceptor Complexes: The Case of the Benzene-Tetracyanoethylene Model. International Journal of Molecular Sciences, 2018, 19, 1134. | 1.8 | 7 |
| 12172 | Liposomal Formulations for an Efficient Encapsulation of Epigallocatechin-3-Gallate: An In-Silico/Experimental Approach. Molecules, 2018, 23, 441. | 1.7 | 23 |
| 12173 | Understanding the Molecule-Electrode Interface for Molecular Spintronic Devices: A Computational and Experimental Study. Molecules, 2018, 23, 1441. | 1.7 | 6 |
| 12174 | Designing High-Refractive Index Polymers Using Materials Informatics. Polymers, 2018, 10, 103. | 2.0 | 31 |
| 12175 | Optimization of the synthesis of a key intermediate for the preparation of glucocorticoids. Steroids, 2018, 137, 14-21. | 0.8 | 3 |
| 12176 | Nonradiative Decay and Stability of <i>N</i> -Heterocyclic Carbene Iridium(III) Complexes. Inorganic Chemistry, 2018, 57, 8881-8889. | 1.9 | 31 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12177 | Catalytic Nitrene Homocoupling by an Iron(II) Bis(alkoxide) Complex: Bulking Up the Alkoxide Enables a Wider Range of Substrates and Provides Insight into the Reaction Mechanism. <i>Inorganic Chemistry</i> , 2018, 57, 9425-9438. | 1.9 | 20 |
| 12178 | Torsional Potentials of Glyoxal, Oxalyl Halides, and Their Thiocarbonyl Derivatives: Challenges for Popular Density Functional Approximations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4806-4817. | 2.3 | 10 |
| 12179 | Quantitative studies on the <i>p</i> -substituent effect of the phenolic component on the polymerization of benzoxazines. <i>Polymer Chemistry</i> , 2018, 9, 4194-4204. | 1.9 | 36 |
| 12180 | cPCET versus HAT: A Direct Theoretical Method for Distinguishing X-H Bond Activation Mechanisms. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 11913-11917. | 7.2 | 77 |
| 12181 | Neutral, Cationic and Hydride-substituted Siloxygermylenes. <i>Chemistry - A European Journal</i> , 2018, 24, 14392-14399. | 1.7 | 44 |
| 12182 | Crystallographic and Computational Studies of Non-Covalent Interactions of Molecular Clips with a Series of Small Solvent Molecules. <i>Journal of Chemical Crystallography</i> , 2018, 48, 131-137. | 0.5 | 1 |
| 12183 | Iodine-Catalyzed Metal-Free Oxidative Ring Opening of Aryltetrahydrocarbolines: Facile Synthesis of α -Aroyl and Aryl Methanimino Indole Derivatives. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 4776-4786. | 1.2 | 6 |
| 12184 | Hormesis of mercuric chloride-human serum albumin adduct on N9 microglial cells via the ERK/MAPKs and JAK/STAT3 signaling pathways. <i>Toxicology</i> , 2018, 408, 62-69. | 2.0 | 13 |
| 12185 | Synthesis, electronic structure and redox properties of the diruthenium sandwich complexes $[\text{Cp}^*\text{Ru}(\text{C}_{10}\text{H}_8)\text{RuCp}^*]^{x+}$ ($x = 0, 1+$; $\text{Cp}^* = \text{C}_5\text{Me}_5$). <i>Journal of Organometallic Chemistry</i> , 2018, 47, 11058-11069. | 1.6 | 5 |
| 12186 | Role of cationic groups on structural and dynamical correlations in hydrated quaternary ammonium-functionalized poly(<i>p</i> -phenylene oxide)-based anion exchange membranes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19350-19362. | 1.3 | 27 |
| 12187 | Molecular dynamics and electronic structure study of neutral, cationic and anionic $(\text{Fe}_3\text{O}_4)^{5-}$ clusters. <i>Chemical Physics Letters</i> , 2018, 706, 494-500. | 1.2 | 9 |
| 12188 | Effect of fluorine substitution of the η^2 -ketoiminate ancillary ligand on photophysical properties and electroluminescence ability of new iridium(C^3) complexes. <i>Journal of Materials Chemistry C</i> , 2018, 6, 8688-8708. | 2.7 | 8 |
| 12189 | Electronic Properties of Vanadium Atoms Adsorption on Clean and Graphene-Covered Cu(111) Surface. <i>Nanoscale Research Letters</i> , 2018, 13, 199. | 3.1 | 4 |
| 12190 | Covalency and Ionicity Do Not Oppose Each Other—Relationship Between Si ⁺ O Bond Character and Basicity of Siloxanes. <i>Chemistry - A European Journal</i> , 2018, 24, 15275-15286. | 1.7 | 40 |
| 12191 | Oxidopyrylium-Alkene [5 + 2] Cycloaddition Conjugate Addition Cascade (C^3) Sequences: Scope, Limitation, and Computational Investigations. <i>Journal of Organic Chemistry</i> , 2018, 83, 9818-9838. | 1.7 | 19 |
| 12192 | Molecular Dynamics Simulation of Water-Based Fracturing Fluids in Kaolinite Slit Pores. <i>Journal of Physical Chemistry C</i> , 2018, 122, 17170-17183. | 1.5 | 33 |
| 12193 | Machine learning meets volcano plots: computational discovery of cross-coupling catalysts. <i>Chemical Science</i> , 2018, 9, 7069-7077. | 3.7 | 154 |
| 12194 | Fluorination of Black Phosphorus—Will Black Phosphorus Burn Down in the Elemental Fluorine?. <i>Advanced Functional Materials</i> , 2018, 28, 1801438. | 7.8 | 34 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12195 | New mono- and dinuclear complexes of 7-azaindole-3-carboxaldehyde with palladium(II): crystal structure, IR and Raman spectra, DFT calculations and in vitro antiproliferative activity. <i>Polyhedron</i> , 2018, 153, 88-98. | 1.0 | 13 |
| 12196 | Asymmetric Synthesis of Diastereo- and Enantiopure Bioxahelicene 2,2'-Bipyridines. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 5164-5178. | 1.2 | 22 |
| 12197 | Time-dependent density functional study of the photoabsorption spectrum of Au ₂₅ (SC ₂ H ₄ C ₆ H ₅) ₁₈ anion: Validation of the computational protocol. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25769. | 1.0 | 9 |
| 12198 | Syntheses of Substituted 1,4-Disila-2,5-cyclohexadienes from Cyclic Hexasilane Si ₆ Me ₁₂ and Alkynes via Successive Si-Si Bond Activation by Pd/Isocyanide Catalysts. <i>Organometallics</i> , 2018, 37, 2531-2543. | 1.1 | 11 |
| 12199 | [Cu ₄ I ₇ 3 ⁻] _n : A novel 1-D iodocuprate aggregate. <i>Journal of Molecular Structure</i> , 2018, 1173, 743-749. | 1.8 | 3 |
| 12200 | A Key Factor Dominating the Competition between Photolysis and Photoracemization of [Ru(bipy) ₃] ₂₊ and [Ru(phen) ₃] ₂₊ Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 8994-9001. | 1.9 | 8 |
| 12201 | Mechanistic insights into hydrodeoxygenation of phenol on bimetallic phosphide catalysts. <i>Catalysis Science and Technology</i> , 2018, 8, 4083-4096. | 2.1 | 31 |
| 12202 | Role of conducting polyaniline interphase on the low field magnetoresistance for LSMO-PANI nanocomposites. <i>Journal of Magnetism and Magnetic Materials</i> , 2018, 466, 446-451. | 1.0 | 2 |
| 12203 | Modeling Chemical Reactions by QM/MM Calculations: The Case of the Tautomerization in Fireflies Bioluminescent Systems. <i>Frontiers in Chemistry</i> , 2018, 6, 116. | 1.8 | 12 |
| 12204 | Multiple Hydrogen-Bond Activation in Asymmetric Brønsted Acid Catalysis. <i>Chemistry - A European Journal</i> , 2018, 24, 7718-7723. | 1.7 | 25 |
| 12205 | Electronic structure of binuclear acetylacetonates of boron difluoride. <i>Journal of Molecular Structure</i> , 2018, 1160, 92-100. | 1.8 | 6 |
| 12206 | Isolation of Mn(I) Compounds Featuring a Reduced Bis(imino)pyridine Chelate and Their Relevance to Electrocatalytic Hydrogen Production. <i>Inorganic Chemistry</i> , 2018, 57, 6065-6075. | 1.9 | 14 |
| 12207 | A Computational Investigation of the Uncatalysed and Water-Catalysed Acyl Rearrangements in Ingenol Esters. <i>Australian Journal of Chemistry</i> , 2018, 71, 212. | 0.5 | 4 |
| 12208 | Photo-stability study of a solution-processed small molecule solar cell system: correlation between molecular conformation and degradation. <i>Science and Technology of Advanced Materials</i> , 2018, 19, 194-202. | 2.8 | 12 |
| 12209 | Mechanisms of acetylcholinesterase protection against sarin and soman by adenosine A1 receptor agonist N6-cyclopentyladenosine. <i>Computational Biology and Chemistry</i> , 2018, 75, 74-81. | 1.1 | 7 |
| 12210 | Spectral Analysis of 3-(Adamantan-1-yl)-4-Ethyl-1-[4-Phenylpiperazin-1-yl]Methyl]-1H-1,2,4-Triazole-5(4H)-Thione. <i>Journal of Applied Spectroscopy</i> , 2018, 85, 203-215. | 0.3 | 2 |
| 12211 | Structural and magnetic susceptibility study of an octanuclear Mn(III)-oxo-pyrazolido complex. <i>Polyhedron</i> , 2018, 149, 142-147. | 1.0 | 5 |
| 12213 | A computational investigation on the antioxidant potential of myricetin 3,4-di-O-β-L-rhamnopyranoside. <i>Journal of Molecular Modeling</i> , 2018, 24, 133. | 0.8 | 39 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12214 | Anisotropy of the Proton Momentum Distribution in Water. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6048-6054. | 1.2 | 12 |
| 12215 | Modelling absorption and emission of a <i>meso</i> -aniline-BODIPY based dye with molecular mechanics. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 14537-14544. | 1.3 | 11 |
| 12216 | Structural determinants influencing halogen bonding: a case study on azinesulfonamide analogs of aripiprazole as 5-HT _{1A} , 5-HT ₇ , and D ₂ receptor ligands. <i>Chemistry Central Journal</i> , 2018, 12, 55. | 2.6 | 8 |
| 12217 | New insights into water-soluble and water-coordinated copper 15-metalacrown-5 gadolinium complexes designed for high-field magnetic resonance imaging applications. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4389. | 1.7 | 15 |
| 12218 | A Quantum-Chemical Study of the Adsorption of Pb Atoms on Au(111). <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2018, 54, 161-169. | 0.3 | 2 |
| 12219 | Exploiting Chromophore-Protein Interactions through Linker Engineering To Tune Photoinduced Dynamics in a Biomimetic Light-Harvesting Platform. <i>Journal of the American Chemical Society</i> , 2018, 140, 6278-6287. | 6.6 | 35 |
| 12220 | Valence and charge-transfer optical properties for some Si _n C _m ($n, m \le 12$) clusters: Comparing TD-DFT, complete-basis-limit EOMCC, and benchmarks from spectroscopy. <i>Journal of Chemical Physics</i> , 2018, 148, 174309. | 1.2 | 1 |
| 12221 | An EPR Investigation of Binding Environments by N-Donor Chelating Exchange Resins for Cu Extraction from Aqueous Media. <i>Inorganic Chemistry</i> , 2018, 57, 10857-10866. | 1.9 | 8 |
| 12222 | Local electrophilicity. <i>Journal of Molecular Modeling</i> , 2018, 24, 245. | 0.8 | 21 |
| 12223 | Investigating the Thermal Stability of Organic Thin-Film Transistors and Phototransistors Based on [1-Benzothieno[3,2- <i>b</i>]pyridine]benzothiophene Dimeric Derivatives. <i>Chemistry - A European Journal</i> , 2018, 24, 16595-16602. | 1.7 | 13 |
| 12224 | Ultrafast interligand electron transfer in <i>cis</i> -[Ru(4,4'-dicarboxylate-2,2'-bipyridine) ₂ (NCS) ₂] ⁴⁺ and implications for electron injection limitations in dye sensitized solar cells. <i>Chemical Science</i> , 2018, 9, 7958-7967. | 3.7 | 14 |
| 12225 | Femtosecond infrared spectroscopy reveals the primary events of the ferrioxalate actinometer. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21390-21403. | 1.3 | 24 |
| 12226 | Kinetics of the Reaction of OH with Isoprene over a Wide Range of Temperature and Pressure Including Direct Observation of Equilibrium with the OH Adducts. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7239-7255. | 1.1 | 16 |
| 12227 | Development of Reaction Density Functional Theory and Its Application to Glycine Tautomerization Reaction in Aqueous Solution. <i>Journal of Physical Chemistry C</i> , 2018, 122, 20745-20754. | 1.5 | 21 |
| 12228 | Correlating Optical and Electrical Dipole Moments To Pinpoint Phosphorescent Dye Alignment in Organic Light-Emitting Diodes. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 31541-31551. | 4.0 | 32 |
| 12229 | Computational study on the mechanisms of [2+3] and [2+2] cycloisomerization reaction catalyzed by gold complex. <i>Journal of Organometallic Chemistry</i> , 2018, 874, 63-69. | 0.8 | 8 |
| 12230 | Theoretical Studies of the Zeolite-Y Encapsulated Chlorine-Substituted Copper(II)phthalocyanine Complex on the Formation Glycidol from Allyl Alcohol. <i>ACS Omega</i> , 2018, 3, 9613-9619. | 1.6 | 5 |
| 12231 | The electronic structure and stability of germanium tubes Ge ₃₀ H ₁₂ and Ge ₃₃ H ₁₂ . <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 23467-23479. | 1.3 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12232 | Synthesis of 1-Carboxamide-1,4-dihydropyridazines via Recyclization of Hydroxypyrrrolines with Semicarbazides. <i>Synthesis</i> , 2018, 50, 4982-4988. | 1.2 | 5 |
| 12233 | New candidates for the global minimum of medium-sized silicon clusters: A hybrid DFTB/DFT genetic algorithm applied to Si_n , $n = 8-80$. <i>Journal of Chemical Physics</i> , 2018, 149, 074313. | 1.2 | 11 |
| 12234 | Multiscale Simulation of the Interaction and Adsorption of Ions on a Hydrophobic Graphene Surface. <i>ChemPhysChem</i> , 2018, 19, 2954-2960. | 1.0 | 17 |
| 12235 | Mechanistic exploration of $\text{CpRe}(\text{CO})_3$ -catalyzed coupling of chloromethyloxirane with CO_2 : Unexpected potentials of CO ligands. <i>Molecular Catalysis</i> , 2018, 458, 25-32. | 1.0 | 2 |
| 12236 | Square planar or octahedral after all? The indistinct solvation of platinum(ii). <i>Dalton Transactions</i> , 2018, 47, 13032-13045. | 1.6 | 3 |
| 12237 | Spectroscopic and first-principles calculation studies of the chemical forms of palladium ion in nitric acid solution for development of disposal of high-level radioactive nuclear wastes. <i>AIP Advances</i> , 2018, 8, 045221. | 0.6 | 10 |
| 12238 | DFT Studies on Ni-Mediated C-F Cleavage for the Synthesis of Cyclopentadiene Derivatives. <i>Frontiers in Chemistry</i> , 2018, 6, 319. | 1.8 | 8 |
| 12239 | Nonadiabatic dynamics simulation of photoisomerization mechanism of photoswitch azodicarboxamide: Hydrogen bonding effects. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 367, 236-239. | 2.0 | 7 |
| 12240 | Assessment of Electrocatalytic Performance of Metal-Free C-Doped BN Nanoflakes for Oxygen Reduction and Hydrogen Evolution Reactions: A Comparative Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 21124-21131. | 1.5 | 10 |
| 12241 | Theoretical Study on the Electronic Structures and Charge Transport Properties of a Series of Rubrene Derivatives. <i>Journal of Physical Chemistry C</i> , 2018, 122, 21226-21238. | 1.5 | 16 |
| 12242 | Inorganic-Organic Hybrid Tongue-Mimic for Time-Resolved Luminescent Noninvasive Pattern and Chiral Recognition of Thiols in Biofluids toward Healthcare Monitoring. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 31725-31734. | 4.0 | 28 |
| 12243 | The Mechanism of C-H Bond Oxidation by Aqueous Permanganate. <i>Environmental Science & Technology</i> , 2018, 52, 9845-9850. | 4.6 | 11 |
| 12244 | Evaluation of Common Theoretical Methods for Predicting Infrared Multiphotonic Dissociation Vibrational Spectra of Intramolecular Hydrogen-Bonded Ions. <i>ACS Omega</i> , 2018, 3, 9075-9085. | 1.6 | 38 |
| 12245 | Unveiling the mechanisms and secrets of chemoselectivities in Au-catalyzed diazo-based couplings with aryl unsaturated aliphatic alcohols. <i>Catalysis Science and Technology</i> , 2018, 8, 4450-4462. | 2.1 | 15 |
| 12246 | Colorimetric sensor for the detection of H_2S and its application in molecular half-subtractor. <i>Analytica Chimica Acta</i> , 2018, 1040, 177-186. | 2.6 | 30 |
| 12247 | High-Energy-Level Blue Phosphor for Solution-Processed White Organic Light-Emitting Diodes with Efficiency Comparable to Fluorescent Tubes. <i>IScience</i> , 2018, 6, 128-137. | 1.9 | 46 |
| 12248 | Toward a Predictive Understanding of Phosphine-Catalyzed [3 + 2] Annulation of Allenolates with Acrylate or Imine. <i>Journal of Organic Chemistry</i> , 2018, 83, 9729-9740. | 1.7 | 22 |
| 12249 | First-order properties from internally contracted multireference coupled-cluster theory with particular focus on hyperfine coupling tensors. <i>Journal of Chemical Physics</i> , 2018, 149, 064101. | 1.2 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12250 | Two New Fluorinated Phenol Derivatives Pyridine Schiff Bases: Synthesis, Spectral, Theoretical Characterization, Inclusion in Epichlorohydrin- β -2-Cyclodextrin Polymer, and Antifungal Effect. <i>Frontiers in Chemistry</i> , 2018, 6, 312. | 1.8 | 23 |
| 12251 | Diarylcyclopropane hydroxamic acid inhibitors of histone deacetylase 4 designed by combinatorial approach and QM/MM calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 85, 97-110. | 1.3 | 4 |
| 12252 | Light induced DNA-functionalized TiO ₂ nanocrystalline interface: Theoretical and experimental insights towards DNA damage detection. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2018, 188, 159-176. | 1.7 | 18 |
| 12253 | Mononuclear thorium halide clusters ThX ₄ (X = F, Cl): gas-phase hydrolysis reactions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21184-21193. | 1.3 | 6 |
| 12254 | V-doping in a potential nonlinear optical material Sr ₂ Nb ₂ O ₇ for increasing the SHG response: A first-principles study. <i>Chemical Physics Letters</i> , 2018, 708, 117-122. | 1.2 | 2 |
| 12255 | Surface adsorption and encapsulated storage of H ₂ molecules in a cage-like (MgO) ₁₂ cluster. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 16609-16616. | 3.8 | 8 |
| 12256 | Intersystem Crossing as a Key Component of the Nonadiabatic Relaxation Dynamics of Bithiophene and Terthiophene. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4530-4540. | 2.3 | 17 |
| 12257 | A DFT-based theoretical model for the calculation of spectral profiles of lanthanide M _{4,5} -edge x-ray absorption. <i>Journal of Chemical Physics</i> , 2018, 149, 054104. | 1.2 | 14 |
| 12258 | Kinetics of the Reaction of the Cyclopentadienyl Radical with Nitrogen Dioxide. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6978-6984. | 1.1 | 0 |
| 12259 | Oxidative dehalogenation and denitration by a flavin-dependent monooxygenase is controlled by substrate deprotonation. <i>Chemical Science</i> , 2018, 9, 7468-7482. | 3.7 | 28 |
| 12260 | On the challenge to improve the density response with unusual gradient approximations. <i>European Physical Journal B</i> , 2018, 91, 1. | 0.6 | 4 |
| 12261 | Transient chirality of anilides - The rotational spectrum of trans-benzanilide. <i>Journal of Molecular Spectroscopy</i> , 2018, 351, 8-13. | 0.4 | 0 |
| 12262 | Accurate Spin-State Energetics for Aryl Carbenes. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4733-4746. | 2.3 | 25 |
| 12263 | An experimental and computational study on isomerically pure, soluble azaphthalocyanines and their complexes and boron azasubphthalocyanines of a varying number of aza units. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 6586-6599. | 1.5 | 13 |
| 12264 | Curvature and vacancies in graphene quantum dots. <i>Applied Surface Science</i> , 2018, 462, 540-548. | 3.1 | 16 |
| 12265 | Electrochemical Generation and Spectroscopic Characterization of the Key Rhodium(III) Hydride Intermediates of Rhodium Poly(bipyridyl) H ₂ -Evolving Catalysts. <i>Inorganic Chemistry</i> , 2018, 57, 11225-11239. | 1.9 | 21 |
| 12266 | Short is strong: experimental electron density in a very short N \cdots I halogen bond. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2018, 233, 733-744. | 0.4 | 17 |
| 12267 | σ -Stereoogenic PN(H)P Iron(II) Catalysts for the Asymmetric Hydrogenation of Ketones: The Importance of Non-Covalent Interactions in Rational Ligand Design by Computation. <i>Advanced Synthesis and Catalysis</i> , 2018, 360, 2900-2913. | 2.1 | 33 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12268 | Expeditious Preparation of Open-Cage Fullerenes by Rhodium(I)-Catalyzed [2+2+2] Cycloaddition of Diynes and C ₆₀ : An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2018, 24, 10653-10661. | 1.7 | 28 |
| 12269 | Synthesis and properties of Fischer carbene complexes of N,N-dimethylaniline and anisole π -coordinated to chromium tricarbonyl. <i>Journal of Organometallic Chemistry</i> , 2018, 869, 54-66. | 0.8 | 7 |
| 12270 | Palladium-Catalyzed Intramolecular C-H Arylation versus 1,5-Palladium Migration: A Theoretical Investigation. <i>Chemistry - an Asian Journal</i> , 2018, 13, 2566-2572. | 1.7 | 19 |
| 12271 | Layer-by-Layer-Assembled AuNPs-Decorated First-Generation Poly(amidoamine) Dendrimer with Reduced Graphene Oxide Core as Highly Sensitive Biosensing Platform with Controllable 3D Nanoarchitecture for Rapid Voltammetric Analysis of Ultratrace DNA Hybridization. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 21541-21555. | 4.0 | 36 |
| 12272 | A prelude to building mathematical models for polypeptide folding: analysis on the conformational potential energy hypersurface cross-sections of N-acetyl-glycyl-glycine-N ^ε -methylamide. <i>Canadian Journal of Chemistry</i> , 2018, 96, 912-921. | 0.6 | 0 |
| 12273 | Electronic Structure and Magnetic Interactions in the Radical Salt [BEDT-TTF] ₂ [CuCl ₄]. <i>Inorganic Chemistry</i> , 2018, 57, 7077-7089. | 1.9 | 5 |
| 12274 | MVO-10: A Gas-Phase Oxide Benchmark for Localization/Delocalization in Mixed-Valence Systems. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3512-3523. | 2.3 | 20 |
| 12275 | Glycerol carbonate as a fuel additive for a sustainable future. <i>Sustainable Energy and Fuels</i> , 2018, 2, 2171-2178. | 2.5 | 38 |
| 12276 | Small phospho-donors phosphorylate MorR without inducing protein conformational changes. <i>Biophysical Chemistry</i> , 2018, 240, 25-33. | 1.5 | 1 |
| 12277 | Structure-activity relationship of xanthates with different hydrophobic groups in the flotation of pyrite. <i>Minerals Engineering</i> , 2018, 125, 155-164. | 1.8 | 32 |
| 12278 | Electron Transfer of Hydrated Transition-Metal Ions and the Electronic State of Co ³⁺ (aq). <i>Inorganic Chemistry</i> , 2018, 57, 7914-7924. | 1.9 | 10 |
| 12279 | Electronic Properties of Free-Standing Surfactant-Capped Lead Halide Perovskite Nanocrystals Isolated in Vacuo. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3604-3611. | 2.1 | 18 |
| 12280 | Polyhedral Trimetallaboranes of the Group 9 Metals: Isocloso versus Capped and Uncapped Closo Deltahedra. <i>Organometallics</i> , 2018, 37, 1845-1851. | 1.1 | 2 |
| 12281 | Computational study of Ru-catalyzed cycloisomerization of 2-alkynylanilides. <i>Journal of Molecular Modeling</i> , 2018, 24, 162. | 0.8 | 4 |
| 12282 | Efficient and Linear-Scaling Seminumeral Method for Local Hybrid Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3451-3458. | 2.3 | 30 |
| 12283 | P-N Bridged Dinuclear Rh-METAMORPhos Complexes: NMR and Computational Studies. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 3761-3769. | 1.0 | 2 |
| 12284 | Analyzing ZnO clusters through the density-functional theory. <i>Journal of Molecular Modeling</i> , 2018, 24, 164. | 0.8 | 9 |
| 12285 | Simple voltammetric analyses of ochratoxin A in food samples using highly-stable and anti-fouling black phosphorene nanosensor. <i>Electrochimica Acta</i> , 2018, 282, 490-498. | 2.6 | 60 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 12286 | Multiferroism and magnetic ordering in new NiBO ₃ (B ²⁺ =Ti, Ge, Zr, Sn, Hf and Pb) materials: A DFT study. <i>Journal of Magnetism and Magnetic Materials</i> , 2018, 465, 412-420. | 1.0 | 13 |
| 12287 | Interplay between hydrogen bonding and n ⁺ π* interaction in an analgesic drug salicin. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18361-18373. | 1.3 | 14 |
| 12288 | Predicting vapor liquid equilibria using density functional theory: A case study of argon. <i>Journal of Chemical Physics</i> , 2018, 148, 224501. | 1.2 | 10 |
| 12289 | Vibrational and electronic absorption spectroscopic profiling, natural hybrid orbital, charge transfer, electron localization function and molecular docking analysis on 3-amino-3-(2-nitrophenyl) propionic acid. <i>Journal of Molecular Structure</i> , 2018, 1171, 733-746. | 1.8 | 32 |
| 12290 | Effect of DNA Environment on Electronically Excited States of Methylene Blue Evaluated by a Three-Layered QM/QM/MM ONIOM Scheme. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4298-4308. | 2.3 | 16 |
| 12291 | The limited extent of the electronic modulation of chlorins and bacteriochlorins through chromene-annulation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18233-18240. | 1.3 | 4 |
| 12292 | Maximising the hydrogen evolution activity in organic photocatalysts by co-polymerisation. <i>Journal of Materials Chemistry A</i> , 2018, 6, 11994-12003. | 5.2 | 93 |
| 12293 | Conformational study of melamine crosslinkers and spectroscopical comparison of HMMM molecules by practical measurements and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2018, 1166, 456-469. | 1.8 | 3 |
| 12294 | Accuracy of TD-DFT Geometries: A Fresh Look. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3715-3727. | 2.3 | 74 |
| 12295 | Comparison of Structures and Energies of Metal Complexes Coordinated with Hydroxyoxime and Carboxylic Acid Extractants by Using Molecular Simulations. <i>Solvent Extraction Research and Development</i> , 2018, 25, 59-69. | 0.5 | 4 |
| 12296 | Crystal structure analysis of a star-shaped triazine compound: a combination of single-crystal three-dimensional electron diffraction and powder X-ray diffraction. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2018, 74, 287-294. | 0.5 | 1 |
| 12297 | Electron Delocalization of Mixed Valence Diiron Sites Mediated by Group 10 Metal Ions in Heterotrimetallic Fe ₂ MFe (M=Ni, Pd, and Pt) Chain Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 11649-11666. | 1.7 | 17 |
| 12298 | Exploring the conformational space of cobalt(III)-salen catalyst for CO ₂ /epoxide copolymerization: Effect of quaternary ammonium salts on preference of alternative isomers. <i>Journal of Computational Chemistry</i> , 2018, 39, 1854-1867. | 1.5 | 11 |
| 12299 | N ₂ O ₅ at water surfaces: binding forces, charge separation, energy accommodation and atmospheric implications. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17961-17976. | 1.3 | 18 |
| 12300 | Magnetic Properties of Mononuclear Co(II) Complexes with Carborane Ligands. <i>Inorganic Chemistry</i> , 2018, 57, 7763-7769. | 1.9 | 14 |
| 12301 | A novel mechanism of heme degradation to biliverdin studied by QM/MM and QM calculations. <i>Dalton Transactions</i> , 2018, 47, 8283-8291. | 1.6 | 9 |
| 12302 | Simulating X-ray Spectroscopies and Calculating Core-Excited States of Molecules. <i>Chemical Reviews</i> , 2018, 118, 7208-7248. | 23.0 | 214 |
| 12303 | Water Dissociation of a Dinuclear Bis(3,5-dimethylpyrazolyl)methane Copper(II) Complex: X-ray Diffraction Structure, Magnetic Properties, and Characteristic Absorption of the (CuN ₂ Cl ₂) ₂ Core. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 3644-3651. | 1.0 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12304 | Range-Separated Double-Hybrid Functional from Nonempirical Constraints. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4052-4062. | 2.3 | 45 |
| 12305 | An intricate balance of hydrogen bonding, ion atmosphere and dynamics facilitates a seamless uracil to cytosine substitution in the U-turn of the neomycin-sensing riboswitch. <i>Nucleic Acids Research</i> , 2018, 46, 6528-6543. | 6.5 | 26 |
| 12306 | New Ru(II) half sandwich complexes bearing the N,Nâ€² bidentate 9-ethyl-N-(pyridin-2-ylmethylene)9H-carbazole-3-amine ligand: Effects of halogen (Clâˆ³, Brâˆ³ and Iâˆ³) leaving groups versus in vitro activity on HepG2 cancer cells, cell cycle, fluorescence study, cellular accumulation and DFT study. <i>Polyhedron</i> , 2018, 152, 37-48. | 1.0 | 3 |
| 12307 | Thermodynamic assessment of carbazole-based organic polycyclic compounds for hydrogen storage applications via a computational approach. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 12158-12167. | 3.8 | 22 |
| 12308 | Synthesis, spectral characterization, DFT computational studies and inhibitory activity of novel N 2 S 2 tetradentates Schiff bases on metallo-beta-lactamases of <i>Acinetobacter baumannii</i> . <i>Journal of Molecular Structure</i> , 2018, 1171, 672-681. | 1.8 | 13 |
| 12309 | Copper (<sc>i>/sc>) dimers stabilized by bis(phenol) amine ligands: theoretical and experimental insights. <i>New Journal of Chemistry</i> , 2018, 42, 12621-12631. | 1.4 | 12 |
| 12310 | Neural-network Kohn-Sham exchange-correlation potential and its out-of-training transferability. <i>Journal of Chemical Physics</i> , 2018, 148, 241737. | 1.2 | 60 |
| 12311 | Regioâ€”and Stereoselective Synthesis of Bicyclic Limoneneâ€”Based Chiral Aminodiols and Spirooxazolidines. <i>Chemistry - A European Journal</i> , 2018, 24, 13607-13615. | 1.7 | 6 |
| 12312 | Panchromatic Sensitization with Zn II Porphyrinâ€”Based Photosensitizers for Lightâ€”Driven Hydrogen Production. <i>ChemSusChem</i> , 2018, 11, 2517-2528. | 3.6 | 30 |
| 12313 | Acido-triggered switching of the second-order nonlinear optical properties of a ferrocenyl-containing indolino-oxazolidine derivative. <i>Dyes and Pigments</i> , 2019, 160, 641-646. | 2.0 | 19 |
| 12314 | An unusual werner type clathrate of Mn(II) benzoate involving energetically significant weak C Hâ€”C contacts: A combined experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2019, 1175, 130-138. | 1.8 | 29 |
| 12315 | How to treat Câ€”F stretching vibrations? A vibrational CD study on chiral fluorinated molecules. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3506-3511. | 1.3 | 36 |
| 12316 | Vibrational properties and bonding analysis of copper hexacyanoferrate complexes in solid state. <i>Applied Spectroscopy Reviews</i> , 2019, 54, 369-424. | 3.4 | 9 |
| 12317 | Microfriction correction factor to the Stokesâ€”Einstein equation for small molecules determined by NMR diffusion measurements and hydrodynamic modelling. <i>Molecular Physics</i> , 2019, 117, 868-876. | 0.8 | 4 |
| 12318 | Broken Symmetry Approach to Magnetic Properties of Oligonuclear Transition-Metal Complexes: Application to Hyperfine Tensors of Mixed-Valence Manganese Compounds. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7717-7730. | 1.5 | 8 |
| 12319 | Synthesis, spectral characterization, crystallographic analysis, DFT studies, bioevaluation and anion exchange reactions of 1-(3-chlorophenyl)-4-(3-phenylseleno propyl) piperazinium chloride. <i>Journal of Molecular Structure</i> , 2019, 1176, 117-127. | 1.8 | 7 |
| 12320 | PySCF-NAO: An efficient and flexible implementation of linear response time-dependent density functional theory with numerical atomic orbitals. <i>Computer Physics Communications</i> , 2019, 236, 188-204. | 3.0 | 8 |
| 12321 | Combined spectroscopic and quantum chemical approach to study the effect of hydrogen bonding interactions in ezetimibe. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 206, 246-253. | 2.0 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12322 | Density functional and ab initio study of samarium dihalides, SmX ₂ (X = I, Br, and Cl). <i>Molecular Physics</i> , 2019, 117, 241-250. | 0.8 | 0 |
| 12323 | Experimental and DFT study of the adsorption of N ₂ O on transition ion-exchanged ZSM-5. <i>Catalysis Today</i> , 2019, 327, 177-181. | 2.2 | 23 |
| 12324 | Study of Li Adsorption on Graphdiyne Using Hybrid DFT Calculations. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 2677-2683. | 4.0 | 33 |
| 12325 | Topological analysis of the electron localisation function (ELF) applied to the electronic structure of oxaziridine: the nature of N-O bond. <i>Structural Chemistry</i> , 2019, 30, 2181-2189. | 1.0 | 27 |
| 12326 | Toward Atomistic Modeling of Irreversible Covalent Inhibitor Binding Kinetics. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3955-3967. | 2.5 | 23 |
| 12327 | Thermochemistry of Guanine Tautomers Re-Examined by Means of High-Level CCSD(T) Composite Ab Initio Methods. <i>Australian Journal of Chemistry</i> , 2019, 72, 607. | 0.5 | 13 |
| 12328 | Complementary Synthetic Approaches toward 9-Phosphatriptycene and Structure-Activity Investigations of Its Association with Sterically Hindered Lewis Acids. <i>Journal of Organic Chemistry</i> , 2019, 84, 11268-11274. | 1.7 | 15 |
| 12329 | A series of silver doped butterfly-like Ti ₈ Ag ₂ clusters with two Ag ions panelled on a Ti ₈ surface. <i>Dalton Transactions</i> , 2019, 48, 13423-13429. | 1.6 | 26 |
| 12330 | Automatic basis-set adaptation in projection-based embedding. <i>Journal of Chemical Physics</i> , 2019, 150, 184104. | 1.2 | 29 |
| 12331 | Angular dependence of strong field ionization of N ₂ by time-dependent configuration interaction using density functional theory and the Tamm-Dancoff approximation. <i>Journal of Chemical Physics</i> , 2019, 151, . | 1.2 | 15 |
| 12332 | Unexpected Bisboronic Dicationic Acid Obtained from One-Pot Condensation Reaction of 3-Aminophenylboronic Acid and 2,6-Pyridinecarboxaldehyde. <i>ChemistrySelect</i> , 2019, 4, 8822-8828. | 0.7 | 1 |
| 12333 | Computational procedure to an accurate DFT simulation to solid state systems. <i>Computational Materials Science</i> , 2019, 170, 109176. | 1.4 | 17 |
| 12334 | Insight into the self-assembly of water-soluble perylene bisimide derivatives through a combined computational and experimental approach. <i>Nanoscale</i> , 2019, 11, 15917-15928. | 2.8 | 13 |
| 12335 | Vibrational spectroscopic characterization, electronic absorption, optical nonlinearity computation and terahertz investigation of (2E)-3-(4-ethoxyphenyl)-1-(3-bromophenyl) prop-2-en-1-one for NLO device fabrication. <i>Journal of Molecular Structure</i> , 2019, 1198, 126909. | 1.8 | 5 |
| 12336 | Theoretical Investigation of Excited-State Intramolecular Proton Transfer and Photoisomerization of 2-(1-methyl)phenol. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7246-7254. | 1.1 | 5 |
| 12337 | Fluorescence of a chiral pentaphene derivative derived from the hexabenzocoronene Motif. <i>Chemical Communications</i> , 2019, 55, 10515-10518. | 2.2 | 5 |
| 12338 | Stabilization of different redox levels of a tridentate benzoxazole amidophenoxide ligand when bound to Co(III) or V(V). <i>Dalton Transactions</i> , 2019, 48, 13326-13336. | 1.6 | 7 |
| 12339 | Delineating the Role of Substituents on the Coordination Behavior of Aroylhydrazone Ligands in Pd ^{II} Complexes and their Influence on Suzuki-Miyaura Coupling in Aqueous Media. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 3869-3882. | 1.0 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12340 | Chemoselectivity in the Oxidation of Cycloalkenes with a Non-Heme Iron(IV)-Oxo-Chloride Complex: Epoxidation vs. Hydroxylation Selectivity. <i>Journal of the American Society for Mass Spectrometry</i> , 2019, 30, 1923-1933. | 1.2 | 9 |
| 12341 | The Fragmentation Dynamics of Simple Organic Molecules of Astrochemical Interest Interacting with VUV Photons. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 1862-1872. | 1.2 | 3 |
| 12342 | Vacuum ultraviolet absorbance of alkanes: an experimental and theoretical investigation. <i>Structural Chemistry</i> , 2019, 30, 2217-2224. | 1.0 | 17 |
| 12343 | Crown Ethers as Electrolyte Additives To Modulate the Electrochemical Potential of Lithium Organic Batteries. <i>Journal of Physical Chemistry C</i> , 2019, 123, 21950-21958. | 1.5 | 6 |
| 12344 | Density Functional Theory Study of the Mechanisms of Iron-Catalyzed Regioselective Anti-Markovnikov Addition of C-H Bonds in Aromatic Ketones to Alkenes. <i>Applied Organometallic Chemistry</i> , 2019, 33, e5183. | 1.7 | 9 |
| 12345 | Mononuclear Ru(II) Complexes of an Arene and Asymmetrically Substituted 2,2'-Bipyridine Ligands: Photophysics, Computation, and NLO Properties. <i>Inorganic Chemistry</i> , 2019, 58, 11470-11479. | 1.9 | 12 |
| 12346 | (±)-Alternariolactones A and B, Two Antiparasitic Alternariol-like Dimers from the Fungus <i>Alternaria alternata</i> P1210 Isolated from the Halophyte <i>Salicornia</i> sp.. <i>Journal of Organic Chemistry</i> , 2019, 84, 11203-11209. | 1.7 | 17 |
| 12347 | Surface-Plasmon-Induced Ammonia Decomposition on Copper: Excited-State Reaction Pathways Revealed by Embedded Correlated Wavefunction Theory. <i>ACS Nano</i> , 2019, 13, 9944-9957. | 7.3 | 38 |
| 12348 | Mechanistic understanding of catalysis by combining mass spectrometry and computation. <i>Chemical Communications</i> , 2019, 55, 12749-12764. | 2.2 | 25 |
| 12349 | Peroxo-Cerium(IV)-Containing Polyoxometalates: [Ce ^{IV} ₆ (O ₂) ₉ (GeW ₁₀ O ₃₇) ₃] ²⁴⁻ a Recyclable Homogeneous Oxidation Catalyst. <i>Inorganic Chemistry</i> , 2019, 58, 11300-11307. | | |
| 12350 | 9-Cobalt(II)-Containing 27-Tungsto-3-germanate(IV): Synthesis, Structure, Computational Modeling, and Heterogeneous Water Oxidation Catalysis. <i>Inorganic Chemistry</i> , 2019, 58, 11308-11316. | 1.9 | 23 |
| 12351 | Aromaticity Suppression by Intermolecular Coordination. Optical Spectra and Electronic Structure of Heavy Carbene Analogues with an Amidophenolate Backbone. <i>Organometallics</i> , 2019, 38, 3174-3180. | 1.1 | 16 |
| 12352 | Statistically representative databases for density functional theory <i>via</i> data science. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19092-19103. | 1.3 | 20 |
| 12353 | Reductive Amination of Ketones with Benzylamine Over Gold Supported on Different Oxides. <i>Catalysis Letters</i> , 2019, 149, 3432-3446. | 1.4 | 10 |
| 12354 | Alkylation of 2-oxo(thioxo)-thieno[2,3-d]pyrimidine-4-ones: Experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2019, 1198, 126858. | 1.8 | 16 |
| 12355 | Photochromic Properties of Novel One-pot Multicomponent Synthesized Tetraarylimidazoles. <i>ChemistrySelect</i> , 2019, 4, 8470-8476. | 0.7 | 10 |
| 12356 | Ab Initio Study of the Stepwise versus Concerted Fragmentation Pathways in Microhydrated Thymine Radical Cations. <i>Chemistry - A European Journal</i> , 2019, 25, 15525-15534. | 1.7 | 3 |
| 12357 | Nickel(II) Complexes with Redox Noninnocent Octaazamacrocycles as Catalysts in Oxidation Reactions. <i>Inorganic Chemistry</i> , 2019, 58, 11133-11145. | 1.9 | 16 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12358 | On the magnetic properties of nanodiamonds: Electronic χ -tensor calculations. <i>Journal of Chemical Physics</i> , 2019, 151, 044305. | 1.2 | 4 |
| 12359 | Potential strategy used for controlling the phosphorescent properties in tetradentate Pt(II) complexes: Effect of azole ligand. <i>Applied Organometallic Chemistry</i> , 2019, 33, e5125. | 1.7 | 2 |
| 12360 | Balancing Donor–Acceptor and Dispersion Effects in Heavy Main Group Element π –Interactions: Effect of Substituents on the Pnictogen– π –Arene Interaction. <i>ChemPhysChem</i> , 2019, 20, 2539-2552. | 1.0 | 10 |
| 12361 | On the formation of propylene oxide from propylene in space: gas-phase reactions. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1. | 0.5 | 3 |
| 12362 | Time-Resolved Infrared and Visible Spectroscopy on Cryptochrome aCRY: Basis for Red Light Reception. <i>Biophysical Journal</i> , 2019, 117, 490-499. | 0.2 | 8 |
| 12363 | M11plus: A Range-Separated Hybrid Meta Functional with Both Local and Rung-3.5 Correlation Terms and High Across-the-Board Accuracy for Chemical Applications. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4804-4815. | 2.3 | 24 |
| 12364 | Enhancing the photo-efficacy of an organic visible-light-activated chromophore (alizarin red S) on zinc oxide with a Ag–Na electrolyte to photo-transform aromatic and aliphatic alcohols. <i>RSC Advances</i> , 2019, 9, 24259-24266. | 1.7 | 5 |
| 12365 | Rethinking CO adsorption on transition-metal surfaces: Effect of density-driven self-interaction errors. <i>Physical Review B</i> , 2019, 100, . | 1.1 | 44 |
| 12366 | Calculating the Gibbs Energies of Solvation of 2,2'-Dipyridyl in Nonaqueous Solvents. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 1206-1208. | 0.1 | 1 |
| 12367 | Electron enrichment of zigzag edges in armchair-oriented graphene nano-ribbons increases their stability and induces pinning of the Fermi level. <i>Carbon</i> , 2019, 154, 211-218. | 5.4 | 7 |
| 12368 | Theoretical Studies on Mild Steel Corrosion Inhibition by 5-Substituted 1H-Tetrazoles in Acidic Media. <i>International Journal of Electrochemical Science</i> , 2019, 14, 2743-2756. | 0.5 | 7 |
| 12369 | The Design of Quaternary Nitrogen Redox Center for High-Performance Organic Battery Materials. <i>Matter</i> , 2019, 1, 945-958. | 5.0 | 71 |
| 12370 | The 4-Electron Cleavage of a N=N Double Bond by a Trimetallic TiNi ₂ Complex. <i>Inorganic Chemistry</i> , 2019, 58, 11762-11772. | 1.9 | 11 |
| 12371 | Azulichlorins and Benzocarbchlorins Derived Therefrom. <i>Journal of Organic Chemistry</i> , 2019, 84, 11649-11664. | 1.7 | 10 |
| 12372 | Toward a Quantum-Chemical Benchmark Set for Enzymatically Catalyzed Reactions: Important Steps and Insights. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7057-7074. | 1.1 | 19 |
| 12373 | Rational Design of Azole-Based Deep Eutectic Solvents for Highly Efficient and Reversible Capture of Ammonia. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 14170-14179. | 3.2 | 62 |
| 12374 | Electronic spectra of flavin in different redox and protonation states: a computational perspective on the effect of the electrostatic environment. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16526-16537. | 1.3 | 33 |
| 12375 | Kinetic hydricity of silane hydrides in the gas phase. <i>Chemical Science</i> , 2019, 10, 8002-8008. | 3.7 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12376 | QM/MM Study of the Uracil DNA Glycosylase Reaction Mechanism: A Competition between Asp145 and His148. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4344-4350. | 2.3 | 11 |
| 12377 | Large-Scale Benchmark of Exchange-Correlation Functionals for the Determination of Electronic Band Gaps of Solids. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5069-5079. | 2.3 | 151 |
| 12378 | Observation of Ultrafast Intersystem Crossing in Thymine by Extreme Ultraviolet Time-Resolved Photoelectron Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6897-6903. | 1.1 | 29 |
| 12379 | The Chemical Bond between Transition Metals and Oxygen: Electronegativity, d-Orbital Effects, and Oxophilicity as Descriptors of Metal-Oxygen Interactions. <i>Journal of Physical Chemistry C</i> , 2019, 123, 18432-18444. | 1.5 | 92 |
| 12380 | Analysis of the Molecular Interactions between Cytochromes P450 3A4 and 1A2 and Aflatoxins: A Docking Study. <i>Applied Sciences (Switzerland)</i> , 2019, 9, 2467. | 1.3 | 4 |
| 12381 | Reactivity of lignin subunits: the influence of dehydrogenation and formation of dimeric structures. <i>Journal of Molecular Modeling</i> , 2019, 25, 228. | 0.8 | 28 |
| 12382 | Evidence of two-state reactivity in water oxidation catalyzed by polyoxometalate-based complex [Mn ₃ (H ₂ O) ₃ (SbW ₉ O ₃₃) ₂] ¹²⁻ . <i>Journal of Catalysis</i> , 2019, 376, 146-149. | 3.1 | 13 |
| 12383 | Probing the Electronic Structure and Chemical Bonding of Uranium Nitride Complexes of NU-XO (X =) Tj ETQq1 1_0.784314 rgBT / Ov | 1.1 | 5 |
| 12384 | Characterization of Molybdenum Dithiocarbamates by First-Principles Calculations. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7007-7015. | 1.1 | 17 |
| 12385 | Importance of Conformational Change in Excited States for Efficient Thermally Activated Delayed Fluorescence. <i>Journal of Physical Chemistry C</i> , 2019, 123, 19322-19332. | 1.5 | 26 |
| 12386 | Cost-effective density functional theory (DFT) calculations of equilibrium isotopic fractionation in large organic molecules. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17555-17570. | 1.3 | 11 |
| 12387 | CO ₂ sorption in triethyl(butyl)phosphonium 2-cyanopyrrolide ionic liquid via first principles simulations. <i>Journal of Molecular Liquids</i> , 2019, 292, 111323. | 2.3 | 7 |
| 12388 | A revised nuclear quadrupole moment for aluminum: Theoretical nuclear quadrupole coupling constants of aluminum compounds. <i>Journal of Chemical Physics</i> , 2019, 150, 224302. | 1.2 | 8 |
| 12389 | A quantitative uncertainty metric controls error in neural network-driven chemical discovery. <i>Chemical Science</i> , 2019, 10, 7913-7922. | 3.7 | 129 |
| 12390 | Synthesis, structure, and properties of EuErCuS ₃ . <i>Journal of Alloys and Compounds</i> , 2019, 805, 779-788. | 2.8 | 12 |
| 12391 | Ï%B2PLYP and Ï%B2GPPLYP: The First Two Double-Hybrid Density Functionals with Long-Range Correction Optimized for Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4735-4744. | 2.3 | 107 |
| 12392 | 47,49Ti solid-state NMR and DFT study of Ziegler-Natta catalyst: Adsorption of TiCl ₄ molecule onto the surface of MgCl ₂ . <i>Journal of Physics and Chemistry of Solids</i> , 2019, 135, 109088. | 1.9 | 14 |
| 12393 | Underestimated Noncovalent Interactions in Protein Data Bank. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3389-3399. | 2.5 | 25 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12394 | Sm-Catalyzed Synthesis and Biological Activity of Acyclic and Cyclic Azadiperoxides. Russian Journal of Organic Chemistry, 2019, 55, 620-632. | 0.3 | 13 |
| 12395 | Dynamic Conformational Behavior in Stable Pentaorganosilicates. European Journal of Inorganic Chemistry, 2019, 2019, 3318-3328. | 1.0 | 4 |
| 12396 | Crystal packing of a zinc(II)-azide complex with a N,N,S-tridentate thiosemicarbazone ligand: An experimental and computational study. Journal of Molecular Structure, 2019, 1197, 393-400. | 1.8 | 9 |
| 12397 | Taming conformational heterogeneity in and with vibrational circular dichroism spectroscopy. Chemical Science, 2019, 10, 7680-7689. | 3.7 | 40 |
| 12398 | Alkylthio- and alkyl-substituted asymmetric diphenyldiacetylene-based liquid crystals: phase transitions, mesophase and single-crystal structures, and birefringence. Liquid Crystals, 2019, 46, 1621-1630. | 0.9 | 17 |
| 12399 | Directed Evolution of P450 BM3 towards Functionalization of Aromatic O-Heterocycles. International Journal of Molecular Sciences, 2019, 20, 3353. | 1.8 | 14 |
| 12400 | The influence of water molecules on the stability of mineral green pigments in Chinese ancient painting. Chemical Physics Letters, 2019, 731, 136592. | 1.2 | 5 |
| 12401 | Ab initio kinetics of the C2H2 + NH2 reaction: a revisited study. Physical Chemistry Chemical Physics, 2019, 21, 17232-17239. | 1.3 | 12 |
| 12402 | Electron transfer and intersystem crossing triggered fluorescence quenching detection of mercury ions. Physical Chemistry Chemical Physics, 2019, 21, 16676-16685. | 1.3 | 7 |
| 12403 | Theoretical investigation of the chiral transition of serine and the roles of water, hydroxyl radical and hydroxide ion. New Journal of Chemistry, 2019, 43, 12340-12350. | 1.4 | 1 |
| 12404 | Solvent effects on acid-base complexes. What is more important: A macroscopic reaction field or solute-solvent interactions?. Journal of Chemical Physics, 2019, 150, 204505. | 1.2 | 17 |
| 12405 | Examining the Factors That Govern the Regioselectivity in Rhodium-Catalyzed Alkyne Cyclotrimerization. Organometallics, 2019, 38, 2853-2862. | 1.1 | 34 |
| 12406 | Theoretical treatment of semiconductor heterojunctions for photocatalysis: the WO ₃ /BiVO ₄ interface. Journal of Physics Condensed Matter, 2019, 31, 434001. | 0.7 | 16 |
| 12407 | Conformational Analyses of Physiological Binary and Ternary Copper(II) Complexes with Asparagine and Histidine; Study of Tridentate Binding of Copper(II) in Aqueous Solution. ChemistryOpen, 2019, 8, 852-868. | 0.9 | 3 |
| 12408 | Density functional study on the thermal stabilities of phenolic bio-oil compounds. Fuel, 2019, 255, 115732. | 3.4 | 12 |
| 12409 | Regioselective synthesis of 2- and 4-diarylpyridine ethers and their inhibitory activities against phosphodiesterase 4B. Journal of Molecular Structure, 2019, 1196, 455-461. | 1.8 | 1 |
| 12410 | Axial Chirality at the Boron-Carbon Bond: Synthesis, Stereodynamic Analysis, and Atropisomeric Resolution of 6-Aryl-5,6-dihydrodibenzo[<i>c,e</i>][1,2]azaborinines. Journal of Organic Chemistry, 2019, 84, 12253-12258. | 1.7 | 20 |
| 12411 | A scaled CIS(D) based method for the calculation of valence and core electron ionization energies. Journal of Chemical Physics, 2019, 151, 034104. | 1.2 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12412 | Metalâ€“Ligand Cooperative Approach To Achieve Dehydrogenative Functionalization of Alcohols to Quinolines and Quinazolin-4(3H)-ones under Mild Aerobic Conditions. <i>Journal of Organic Chemistry</i> , 2019, 84, 10160-10171. | 1.7 | 77 |
| 12413 | On the Accuracy of Density Functional Theory in Zeolite Catalysis. <i>ChemCatChem</i> , 2019, 11, 4368-4376. | 1.8 | 55 |
| 12414 | Thermodynamic and kinetic studies on OH-involved photo-decarboxylation mechanism for waste cooking oils to biofuels. <i>Fuel</i> , 2019, 254, 115665. | 3.4 | 4 |
| 12415 | <i>adj</i> -Dicarbaporphyrinoid Systems: Synthesis, Spectroscopic Characterization, and Reactivity of 23-Carbabenziporphyrins. <i>Journal of Organic Chemistry</i> , 2019, 84, 10237-10256. | 1.7 | 2 |
| 12416 | Captodative Substitution Enhances the Diradical Character of Compounds, Reduces Aromaticity, and Controls Single-Molecule Conductivity Patterns: A Valence Bond Study. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7133-7141. | 1.1 | 12 |
| 12417 | Accurate Binding Energies for Lithium Polysulfides and Assessment of Density Functionals for Lithiumâ€“Sulfur Battery Research. <i>Journal of Physical Chemistry C</i> , 2019, 123, 20737-20747. | 1.5 | 34 |
| 12418 | Hydroalkynylation of Enamides Using Iridium or Rhodium Complexes: DFT Study on the Mechanism and Regioselectivity. <i>Organometallics</i> , 2019, 38, 2998-3006. | 1.1 | 17 |
| 12419 | Polypyrrole derivatives for optoelectronic applications: a DFT study on the influence of side groups. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17729-17739. | 1.3 | 23 |
| 12420 | Heterocycle Effects on the Liquid Crystallinity of Terthiophene Analogues. <i>Materials</i> , 2019, 12, 2314. | 1.3 | 6 |
| 12421 | Cytotoxic Sesquiterpenoid Quinones and Quinols, and an 11-Membered Heterocycle, Kauamide, from the Hawaiian Marine Sponge <i>Dactylospongia elegans</i> . <i>Marine Drugs</i> , 2019, 17, 423. | 2.2 | 14 |
| 12422 | Hierarchy in the Halogen Activation During Surfaceâ€“Promoted Ullmann Coupling. <i>ChemPhysChem</i> , 2019, 20, 2305-2310. | 1.0 | 11 |
| 12423 | Machine Learning Accelerates the Discovery of Design Rules and Exceptions in Stable Metalâ€“Oxo Intermediate Formation. <i>ACS Catalysis</i> , 2019, 9, 8243-8255. | 5.5 | 67 |
| 12424 | Ruthenium-catalysed oxidative conversion of ammonia into dinitrogen. <i>Nature Chemistry</i> , 2019, 11, 702-709. | 6.6 | 75 |
| 12425 | Molecular Vibrations of an Oxygenâ€“Evolving Complex and Its Synthetic Mimic. <i>Chemistry - A European Journal</i> , 2019, 25, 13385-13395. | 1.7 | 2 |
| 12426 | Highly efficient phosphorescence from cyclometallated iridium(III) compounds: Improved syntheses of picolinate complexes and quantum chemical studies of their electronic structures. <i>Inorganica Chimica Acta</i> , 2019, 496, 119040. | 1.2 | 2 |
| 12427 | Optimal transport and colossal ionic mechano-conductance in graphene crown ethers. <i>Science Advances</i> , 2019, 5, eaaw5478. | 4.7 | 37 |
| 12428 | Supercell calculations of the geometry and lattice energy of β -glycine crystal. <i>Journal of Molecular Modeling</i> , 2019, 25, 244. | 0.8 | 3 |
| 12429 | Pd(II) Complexes with Chelating Phosphinoferrocene Diaminocarbene Ligands: Synthesis, Characterization, and Catalytic Use in Pd-Catalyzed Borylation of Aryl Bromides. <i>Organometallics</i> , 2019, 38, 3060-3073. | 1.1 | 13 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12430 | Computational Evidence for Kinetically Controlled Radical Coupling during Lignification. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 13270-13277. | 3.2 | 21 |
| 12431 | Free radical induced selenoxide formation in isomeric organoselenium compounds: the effect of chemical structures on antioxidant activity. <i>New Journal of Chemistry</i> , 2019, 43, 13357-13362. | 1.4 | 13 |
| 12432 | Bilirubin Links Heme Metabolism to Neuroprotection by Scavenging Superoxide. <i>Cell Chemical Biology</i> , 2019, 26, 1450-1460.e7. | 2.5 | 66 |
| 12433 | Mechanistic insight on the chemistry of potential Pt antitumor agents as revealed by collaborative research performed in Kragujevac and Erlangen. <i>Inorganica Chimica Acta</i> , 2019, 495, 118953. | 1.2 | 8 |
| 12434 | Strong Influence of Decoherence Corrections and Momentum Rescaling in Surface Hopping Dynamics of Transition Metal Complexes. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5031-5045. | 2.3 | 50 |
| 12435 | Resonance Raman Spectroscopy and Density Functional Theory Calculations on Ferrous Porphyrin Dioxygen Adducts with Different Axial Ligands: Correlation of Ground State Wave Function and Geometric Parameters with Experimental Vibrational Frequencies. <i>Inorganic Chemistry</i> , 2019, 58, 10704-10715. | 1.9 | 13 |
| 12436 | An Insight on the Gold(I) Affinity of <i>golB</i> Protein via Multilevel Computational Approaches. <i>Inorganic Chemistry</i> , 2019, 58, 11091-11099. | 1.9 | 19 |
| 12437 | Efficient and Reversible SO ₂ Absorption by Environmentally Friendly Task-Specific Deep Eutectic Solvents of PPZBr + Gly. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 14236-14246. | 3.2 | 75 |
| 12438 | Mn(I) and Fe(II)/PN(H)P Catalysts for the Hydrogenation of Ketones: A Comparison by Experiment and Calculation. <i>Advanced Synthesis and Catalysis</i> , 2019, 361, 4691-4706. | 2.1 | 42 |
| 12439 | Origins of the Electronic Modulations of Bacterio- and Isobacteriodilactone Regioisomers. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7470-7485. | 1.1 | 14 |
| 12440 | Computational Assessment of MLCT versus MC Stabilities in First- to Third-Row d ⁶ Pseudo-Octahedral Transition Metal Complexes. <i>Journal of Computational Chemistry</i> , 2019, 40, 2377-2390. | 1.5 | 4 |
| 12441 | A DFT/TDDFT investigation on structure-photophysical properties relationship of phenothiazine derivatives with substitutions on C-3/N-10 sites. <i>Computational and Theoretical Chemistry</i> , 2019, 1163, 112512. | 1.1 | 4 |
| 12442 | Using Ultrafast X-ray Spectroscopy To Address Questions in Ligand-Field Theory: The Excited State Spin and Structure of [Fe(dcpp) ₂] ²⁺ . <i>Inorganic Chemistry</i> , 2019, 58, 9341-9350. | 1.9 | 29 |
| 12443 | Untangling Hydrogen Bond Networks with Ion Mobility Spectrometry and Quantum Chemical Calculations: A Case Study on H ⁺ XPGG. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5730-5741. | 1.2 | 2 |
| 12444 | A two-dimensional MoS ₂ /C ₃ N broken-gap heterostructure, a first principles study. <i>RSC Advances</i> , 2019, 9, 19837-19843. | 1.7 | 32 |
| 12445 | A new approach to predict the formation of 3D hybrid organic-inorganic perovskites. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e26012. | 1.0 | 8 |
| 12446 | Lithium-Aluminate-Catalyzed Hydrophosphination Applications. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 12291-12296. | 7.2 | 40 |
| 12447 | A Computational Study of the Reaction N(2D) ⁺ +C ₆ H ₆ Leading to Pyridine and Phenylnitrene. <i>Lecture Notes in Computer Science</i> , 2019, , 316-324. | 1.0 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12448 | Gold(I)-catalyzed [4+ 1]/[4+ 3] annulations of diazo esters with hexahydro-1,3,5-triazines: Theoretical study of mechanism and regioselectivity. <i>Journal of Organometallic Chemistry</i> , 2019, 897, 70-79. | 0.8 | 5 |
| 12449 | Dependence of the virial exciton model on basis set and exact-exchange fraction. <i>Journal of Chemical Physics</i> , 2019, 150, 241101. | 1.2 | 1 |
| 12450 | Facile Fluorescence Monitoring of Gut Microbial Metabolite Trimethylamine <i>N</i> -oxide via Molecular Recognition of Guanidinium-Modified Calixarene. <i>Theranostics</i> , 2019, 9, 4624-4632. | 4.6 | 41 |
| 12451 | Contribution of substrate reorganization energies of electron transfer to laccase activity. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15805-15814. | 1.3 | 9 |
| 12452 | Hemilabile bonding of 1-oxa-4,7-dithiacyclononane in cyclometallated palladium(ii) complexes. <i>Dalton Transactions</i> , 2019, 48, 11520-11535. | 1.6 | 2 |
| 12453 | Ligand-free Cu(II)-catalyzed aerobic etherification of aryl halides with silanes: an experimental and theoretical approach. <i>New Journal of Chemistry</i> , 2019, 43, 11316-11333. | 1.4 | 6 |
| 12454 | Electronic structures and binding motifs of sodium polysulfide clusters NaSn ⁿ⁻ (n = 5-9): A joint negative ion photoelectron spectroscopy and computational investigation. <i>Journal of Chemical Physics</i> , 2019, 150, 244305. | 1.2 | 4 |
| 12455 | A spectroelectrochemical investigation of the heme-based sensor DevS from <i>Mycobacterium tuberculosis</i> : a redox versus oxygen sensor. <i>FEBS Journal</i> , 2019, 286, 4278-4293. | 2.2 | 11 |
| 12456 | Cross-Comparisons between Experiment, TD-DFT, CC, and ADC for Transition Energies. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4581-4590. | 2.3 | 58 |
| 12457 | Formation of hydroxylated polybrominated diphenyl ethers and hydroxylated polybrominated biphenyls during the adsorption of bromophenols by reduced graphene oxide. <i>Chemical Engineering Journal</i> , 2019, 378, 122134. | 6.6 | 3 |
| 12458 | Lithium-Aluminate-Catalyzed Hydrophosphination Applications. <i>Angewandte Chemie</i> , 2019, 131, 12419-12424. | 1.6 | 12 |
| 12459 | Ascorbigen ¹⁵ NMR identification. <i>Magnetic Resonance in Chemistry</i> , 2019, 57, 1084-1096. | 1.1 | 3 |
| 12460 | Fluorescein ether-ester dyes for labeling of fluorinated methacrylate nanoparticles. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 382, 111956. | 2.0 | 9 |
| 12461 | Conducting copolymers nanocomposite coatings with aggregation-controlled luminescence and efficient corrosion inhibition properties. <i>Progress in Organic Coatings</i> , 2019, 135, 525-535. | 1.9 | 35 |
| 12462 | Theoretical design of porphyrin dyes with electron-deficit heterocycles towards near-IR light sensitization in dye-sensitized solar cells. <i>Solar Energy</i> , 2019, 188, 742-749. | 2.9 | 9 |
| 12463 | Chalcogenide glasses as a playground for the application of first-principles molecular dynamics to disordered materials. <i>Solid State Sciences</i> , 2019, 95, 105925. | 1.5 | 4 |
| 12464 | A computational study on the electronic and optical properties of boron-nitride circumacenes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16302-16309. | 1.3 | 20 |
| 12465 | Determination of the absolute configuration of conformationally flexible molecules by simulation of chiro-optical spectra: a case study. <i>RSC Advances</i> , 2019, 9, 18165-18175. | 1.7 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12466 | Interatomic potentials of Mg ions in aqueous solutions: structure and dehydration kinetics. <i>European Journal of Mineralogy</i> , 2019, 31, 275-287. | 0.4 | 13 |
| 12467 | Chemical Kinetics of Hydrogen Atom Abstraction from Propargyl Sites by Hydrogen and Hydroxy Radicals. <i>International Journal of Molecular Sciences</i> , 2019, 20, 3227. | 1.8 | 6 |
| 12468 | Electronic Structure and Kinetics Calculations for the Si+SH Reaction, a Possible Route of SiS Formation in Star-Forming Regions. <i>Lecture Notes in Computer Science</i> , 2019, , 306-315. | 1.0 | 4 |
| 12469 | Theoretical Studies of Two Key Low-Lying Carbenes of C ₅ H ₂ Missing in the Laboratory. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6618-6627. | 1.1 | 18 |
| 12470 | Two New Cocrystals of the Dipicolinic Acid. Hirshfeld Atom Refinement of Crystal Structures and Quantum Theory of Atoms in Molecules Analysis of Molecular Complexes. <i>Crystal Growth and Design</i> , 2019, 19, 6860-6872. | 1.4 | 5 |
| 12471 | Cyclobutastellettolides A and B, C ₁₉ Norterenoids from a <i>Stelletta</i> sp. Marine Sponge. <i>Journal of Natural Products</i> , 2019, 82, 3196-3200. | 1.5 | 15 |
| 12472 | Gas-Phase and Ionic Liquid Experimental and Computational Studies of Imidazole Acidity and Carbon Dioxide Capture. <i>Journal of Organic Chemistry</i> , 2019, 84, 14593-14601. | 1.7 | 10 |
| 12473 | Free Energy Profile of a Model Palladium Catalyzed Fluorination of Aryl Bromide with Cesium Fluoride. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9850-9856. | 1.1 | 8 |
| 12474 | Activation of Dioxygen by a Mononuclear Nonheme Iron Complex: Sequential Peroxo, Oxo, and Hydroxo Intermediates. <i>Journal of the American Chemical Society</i> , 2019, 141, 17533-17547. | 6.6 | 36 |
| 12475 | Computational Exploration of Chiral Iron Porphyrin-Catalyzed Asymmetric Hydroxylation of Ethylbenzene Where Stereoselectivity Arises from π - π Stacking Interaction. <i>Journal of Organic Chemistry</i> , 2019, 84, 13755-13763. | 1.7 | 10 |
| 12476 | Hypergolic Triggers as Co-crystal Formers: Co-crystallization for Creating New Hypergolic Materials with Tunable Energy Content. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 18399-18404. | 7.2 | 25 |
| 12477 | Self-Assemble and In-situ Formation of Laponite RDS Decorated d-Ti ₃ C ₂ T _x Hybrids for Application in Lithium-Ion Battery. <i>ChemistrySelect</i> , 2019, 4, 10694-10700. | 0.7 | 5 |
| 12478 | Self-healing electromagnetic interference shielding composite based on Diels-Alder chemistry. <i>Journal of Materials Science: Materials in Electronics</i> , 2019, 30, 19994-20001. | 1.1 | 6 |
| 12479 | Coupling Constants, High Spin, and Broken Symmetry States of Organic Radicals: an Assessment of the Molecules-in-Molecules Fragmentation-Based Method. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5998-6009. | 2.3 | 6 |
| 12480 | Oligomer Electrolytes for Light-Emitting Electrochemical Cells: Influence of the End Groups on Ion Coordination, Ion Binding, and Turn-on Kinetics. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 40372-40381. | 4.0 | 7 |
| 12481 | Supramolecular Nanowires from an Acceptor-Donor-Acceptor Conjugated Chromophore. <i>Chemistry - A European Journal</i> , 2019, 25, 16725-16731. | 1.7 | 14 |
| 12482 | Effect of ring size on photoisomerization properties of stiff stilbene macrocycles. <i>Beilstein Journal of Organic Chemistry</i> , 2019, 15, 2408-2418. | 1.3 | 7 |
| 12483 | Structural investigation, Hirshfeld surface analysis, characterization and computational studies of a novel chlorobismuthate(III) complex. <i>Chemical Data Collections</i> , 2019, 24, 100289. | 1.1 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12484 | Cercosporin-bioinspired photoreductive activation of aryl halides under mild conditions. <i>Journal of Catalysis</i> , 2019, 380, 1-8. | 3.1 | 19 |
| 12485 | A detailed computational investigation on the structural and spectroscopic properties of propolisbenzofuran B. <i>Heliyon</i> , 2019, 5, e02518. | 1.4 | 14 |
| 12486 | A Mechanistic Study of a Potent and Selective Epidermal Growth Factor Receptor Inhibitor against the L858R/T790M Resistance Mutation. <i>Biochemistry</i> , 2019, 58, 4246-4259. | 1.2 | 3 |
| 12487 | Assessing density functional theory in real-time and real-space as a tool for studying bacteriochlorophylls and the light-harvesting complex 2. <i>Journal of Chemical Physics</i> , 2019, 151, 134114. | 1.2 | 12 |
| 12488 | The nature of the lead-iodine bond in PbI ₂ : A case study for the modelling of lead halide perovskites. <i>Computational and Theoretical Chemistry</i> , 2019, 1164, 112558. | 1.1 | 9 |
| 12489 | Water-Soluble Chiral Y(III)-Cu(II) Metallamacrocyclic Phenylalaninehydroximate Complex. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2019, 45, 721-727. | 0.3 | 7 |
| 12490 | Hypercoordinated organotin(IV) compounds containing C,O- and C,N- chelating ligands: Synthesis, characterisation, DFT studies and polymerization behaviour. <i>Journal of Organometallic Chemistry</i> , 2019, 900, 120910. | 0.8 | 10 |
| 12491 | Experimental and theoretical analysis on decomposition and by-product formation process of (CF ₃) ₂ CFCN mixture. <i>AIP Advances</i> , 2019, 9, . | 0.6 | 14 |
| 12492 | Pyrazole Compounds : Synthesis, molecular structure, chemical reactivity, experimental and theoretical DFT FTIR spectra. <i>Materials Today: Proceedings</i> , 2019, 13, 956-963. | 0.9 | 7 |
| 12493 | DFT and experimental study of triallylborane-mediated isomerization of $\hat{\pm}$ -allylated azaheterocycles. <i>Mendeleev Communications</i> , 2019, 29, 190-193. | 0.6 | 4 |
| 12494 | Spectroelectrochemical, photochemical and theoretical study of octaazamacrocyclic nickel(II) complexes exhibiting unusual solvent-dependent deprotonation of methylene group. <i>Electrochimica Acta</i> , 2019, 326, 135006. | 2.6 | 5 |
| 12495 | Mapping Microstructural Dynamics up to the Nanosecond of the Conjugated Polymer P3HT in the Solid State. <i>Chemistry of Materials</i> , 2019, 31, 9635-9651. | 3.2 | 10 |
| 12496 | Simple and Efficient Truncation of Virtual Spaces in Embedded Wave Functions via Concentric Localization. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6085-6096. | 2.3 | 27 |
| 12497 | Role of Guanidinium-Carboxylate Ion Interaction in Enzyme Inhibition with Implications for Drug Design. <i>Journal of Physical Chemistry B</i> , 2019, 123, 9302-9311. | 1.2 | 13 |
| 12498 | Mechanism of the Iron(0)-Catalyzed Hydrosilylation of Aldehydes: A Combined DFT and Experimental Investigation. <i>Organometallics</i> , 2019, 38, 4105-4114. | 1.1 | 13 |
| 12499 | Benchmarking DFT-D Dispersion Corrections for Anharmonic Vibrational Frequencies and Harmonic Scaling Factors. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9800-9808. | 1.1 | 16 |
| 12500 | Approximating Periodic Potential Energy Surfaces with Sparse Trigonometric Interpolation. <i>Journal of Physical Chemistry B</i> , 2019, 123, 9677-9684. | 1.2 | 3 |
| 12501 | Study on Short-Circuit Impedance Characteristics in DN Traction Electric Lines. <i>IOP Conference Series: Earth and Environmental Science</i> , 2019, 310, 032053. | 0.2 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12502 | Predicting an Antiaromatic Benzene Ring in the Ground State Caused by Hyperconjugation. Chemistry - an Asian Journal, 2019, 14, 4309-4314. | 1.7 | 5 |
| 12503 | Mechanistic Investigation of Au(III)-Catalyzed Cycloisomerizations of <i>N</i> -Propargylcarboxamides. European Journal of Organic Chemistry, 2019, 2019, 6822-6829. | 1.2 | 3 |
| 12504 | Base-Assisted Conversion of Protonated D-Fructose to 5-HMF: Searching for Gas-Phase Green Models. ChemistryOpen, 2019, 8, 1190-1198. | 0.9 | 10 |
| 12505 | Unexpected Molecular Structure of a Putative Rhenium-Dioxo-Benzocarbaporphyrin Complex. Implications for the Highest Transition Metal Valence in a Porphyrin-Type Ligand Environment. ChemistryOpen, 2019, 8, 1298-1302. | 0.9 | 9 |
| 12506 | Small substituent groups as geometric controllers for tridentate platinum(II) complexes to effectively suppress non-radiative decay processes. Physical Chemistry Chemical Physics, 2019, 21, 2764-2770. | 1.3 | 14 |
| 12507 | Templating metastable Pd ₂ carboxylate aggregates. Chemical Science, 2019, 10, 1823-1830. | 3.7 | 15 |
| 12508 | Higher amounts of loophole-free Bell violation using a heralded entangled source. New Journal of Physics, 2019, 21, 103008. | 1.2 | 3 |
| 12509 | Temperature field modeling of the plate during hot rolling based on inverse heat conduction problem. Journal of Physics: Conference Series, 2019, 1300, 012017. | 0.3 | 0 |
| 12510 | Low Voltage Power Line Communication Routing Method based on Improved Genetic Algorithm. , 2019, , . | | 0 |
| 12511 | Quantum chemical calculations of ³¹ P NMR chemical shifts of P-donor ligands in platinum(II) complexes. Journal of Molecular Modeling, 2019, 25, 329. | 0.8 | 3 |
| 12512 | Oxygen Functional Group Modification of Cellulose-Derived Hard Carbon for Enhanced Sodium Ion Storage. ACS Sustainable Chemistry and Engineering, 2019, 7, 18554-18565. | 3.2 | 72 |
| 12513 | Theoretical Studies of the Hydrogen Abstraction from Poly(oxymethylene) Dimethyl Ethers by O ₂ in Relation with Cetane Number Data. ACS Omega, 2019, 4, 19128-19135. | 1.6 | 3 |
| 12514 | The Myth of d ⁸ Copper(III). Journal of the American Chemical Society, 2019, 141, 18508-18520. | 6.6 | 139 |
| 12515 | What Electronic Structure Method Can Be Used in the Global Optimization of Nanoclusters?. Journal of Physical Chemistry A, 2019, 123, 10454-10462. | 1.1 | 15 |
| 12516 | Predicting Potential Inversion Behavior of Ru-aqua Complexes via Using Cost Effective DFT Calculations. Bulletin of the Korean Chemical Society, 2019, 40, 1098-1111. | 1.0 | 1 |
| 12517 | Luminescence and Electron Dynamics in Atomically Precise Nanoclusters with Eight Superatomic Electrons. Journal of the American Chemical Society, 2019, 141, 18715-18726. | 6.6 | 59 |
| 12518 | Redox-Active Guanidines with One or Two Guanidino Groups and Their Integration in Low-Dimensional Perovskite Structures. European Journal of Inorganic Chemistry, 2019, 2019, 4147-4160. | 1.0 | 5 |
| 12519 | Viewpoint: Atomic-Scale Design Protocols toward Energy, Electronic, Catalysis, and Sensing Applications. Inorganic Chemistry, 2019, 58, 14939-14980. | 1.9 | 23 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12520 | Tools for Prescreening the Most Active Sites on Ir and Rh Clusters toward C-H Bond Cleavage of Ethane: NBO Charges and Wiberg Bond Indexes. ACS Omega, 2019, 4, 18809-18819. | 1.6 | 10 |
| 12521 | Acid selective pro-dye for cellular compartments. Scientific Reports, 2019, 9, 15304. | 1.6 | 10 |
| 12522 | Mechanomagnetics in Elastic Crystals: Insights from [Cu(acac) ₂]. Angewandte Chemie, 2019, 131, 15226-15232. | 1.6 | 10 |
| 12523 | Hydrogen Abstraction from the C15 Position of the Cholesterol Skeleton. Journal of Organic Chemistry, 2019, 84, 15184-15191. | 1.7 | 3 |
| 12524 | Mutations of Triad Determinants Changes the Substrate Alignment at the Catalytic Center of Human ALOX5. ACS Chemical Biology, 2019, 14, 2768-2782. | 1.6 | 13 |
| 12525 | Evaluating Computational Chemistry Methods for Isotopic Fractionation between CO ₂ (g) and H ₂ O(g). Journal of Chemical Information and Modeling, 2019, 59, 4663-4677. | 2.5 | 1 |
| 12526 | Relevance of the Pauli kinetic energy density for semilocal functionals. Physical Review B, 2019, 100, . | 1.1 | 38 |
| 12527 | Emission solvatochromic, solid-state and aggregation-induced emissive 1H-pyridines and emission-tuneable 1H-pyridines by Michael addition-cyclocondensation sequences. Beilstein Journal of Organic Chemistry, 2019, 15, 2684-2703. | 1.3 | 4 |
| 12528 | Rx-COSMO-CAMD: Computer-Aided Molecular Design of Reaction Solvents Based on Predictive Kinetics from Quantum Chemistry. Industrial & Engineering Chemistry Research, 2019, 58, 22835-22846. | 1.8 | 25 |
| 12529 | On Transannulation in Azaphosphatranes: Synthesis and Theoretical Analysis. Inorganic Chemistry, 2019, 58, 15983-15992. | 1.9 | 7 |
| 12530 | Resonant X-ray Sum-Frequency-Generation Spectroscopy of K-Edges in Acetyl Fluoride. Journal of Chemical Theory and Computation, 2019, 15, 6832-6839. | 2.3 | 5 |
| 12531 | Electronic g-tensors of nanodiamonds: Dependence on the size, shape, and surface functionalization. Journal of Chemical Physics, 2019, 151, 144305. | 1.2 | 3 |
| 12532 | Synthesis, Structure and In Vitro Cytotoxic Activity of Novel Cinchona-Chalcone Hybrids with 1,4-Disubstituted- and 1,5-Disubstituted 1,2,3-Triazole Linkers. Molecules, 2019, 24, 4077. | 1.7 | 10 |
| 12533 | Photoswitchable Boronic Acid Derived Salicylidenehydrazone Enabled by Photochromic Spirooxazine and Fulgide Moieties: Multiple Responses of Optical Absorption, Fluorescence Emission, and Quadratic Nonlinear Optics. Journal of Physical Chemistry C, 2019, 123, 29838-29855. | 1.5 | 38 |
| 12534 | Unimolecular Exciplexes by Ugi Four-Component Reaction. Frontiers in Chemistry, 2019, 7, 717. | 1.8 | 2 |
| 12535 | Structural and Optical Properties of Metal-Nitrosyl Complexes. Molecules, 2019, 24, 3638. | 1.7 | 9 |
| 12536 | Quantum Interference and Substantial Property Tuning in Conjugated ortho-Regio-Resistive Organic (ZORRO) Junctions. Nano Letters, 2019, 19, 8956-8963. | 4.5 | 10 |
| 12537 | Electronic Structure of Tetracyanonickelate(II). Inorganic Chemistry, 2019, 58, 15202-15206. | 1.9 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12538 | Effect of β -Ketoiminato Ancillary Ligand Modification on Emissive Properties of New Iridium Complexes. <i>Inorganic Chemistry</i> , 2019, 58, 15671-15686. | 1.9 | 8 |
| 12539 | Enantioselective Synthesis of Isoxazoline <i>N</i> -Oxides via Pd-Catalyzed Asymmetric Allylic Cycloaddition of Nitro-Containing Allylic Carbonates. <i>Organic Letters</i> , 2019, 21, 9045-9049. | 2.4 | 31 |
| 12540 | Theoretical Insight into the Performance of Mn ^{II/III} -Monosubstituted Heteropolytungstates as Water Oxidation Catalysts. <i>Inorganic Chemistry</i> , 2019, 58, 15751-15757. | 1.9 | 11 |
| 12541 | Clusters of betaine with positive and negative ions: Evidence for the betaine tetramer being magic. <i>Journal of Chemical Physics</i> , 2019, 151, 184303. | 1.2 | 1 |
| 12542 | Hypergolic Triggers as Co-crystal Formers: Co-crystallization for Creating New Hypergolic Materials with Tunable Energy Content. <i>Angewandte Chemie</i> , 2019, 131, 18570-18575. | 1.6 | 7 |
| 12543 | Performance of Density Functional Theory for Transition Metal Oxygen Bonds. <i>ChemPhysChem</i> , 2019, 20, 3210-3220. | 1.0 | 9 |
| 12544 | Influence of Steric Hindrance on Ferroelectric and Piezoelectric Performance of Poly(vinylidene fluoride) Terpolymer. <i>Journal of Applied Physics</i> , 2019, 125, 104101. | 1.1 | 17 |
| 12545 | Electron Transfer and Electron Excitation Processes in 2,5-Diaminoterephthalate Derivatives with Broad Scope for Functionalization. <i>ChemistryOpen</i> , 2019, 8, 1176-1182. | 0.9 | 2 |
| 12546 | Synthesis and Characterization of Salts of the 3,6-Dinitro-1,2,4-triazolo[4,3- <i>b</i>][1,2,4]triazolate Anion: Insensitive Energetic Materials Available From Economical Precursors. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2019, 645, 1197-1204. | 0.6 | 16 |
| 12547 | Formation of highly oxygenated multifunctional compounds from cross-reactions of carbonyl compounds in the atmospheric aqueous phase. <i>Atmospheric Environment</i> , 2019, 219, 117046. | 1.9 | 16 |
| 12548 | From gene delivery agents to ionic liquids: The impacts of cation structure and anion identity on liquefaction. <i>Journal of Molecular Liquids</i> , 2019, 296, 111758. | 2.3 | 4 |
| 12549 | Investigating the Microstructure of Poly(cyclosilane) by ²⁹ Si Solid-State NMR Spectroscopy and DFT Calculations. <i>Chemistry of Materials</i> , 2019, 31, 9168-9178. | 3.2 | 16 |
| 12550 | Evaluation of the Tetrakis(3-Hydroxy-4-Pyridinone) Ligand THPN with Zirconium(IV): Thermodynamic Solution Studies, Bifunctionalization, and in Vivo Assessment of Macromolecular 89Zr-THPN-Conjugates. <i>Inorganic Chemistry</i> , 2019, 58, 14667-14681. | 1.9 | 13 |
| 12551 | Band Gap of 3D Metal Oxides and Quasi-2D Materials from Hybrid Density Functional Theory: Are Dielectric-Dependent Functionals Superior?. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6294-6312. | 2.3 | 45 |
| 12552 | Performances of Density Functional Tight-Binding Methods for Describing Ground and Excited State Geometries of Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6267-6276. | 2.3 | 12 |
| 12553 | Donor-Acceptor π -Conjugated Enamines: Functional Group-Compatible Synthesis from Amides and Their Photoabsorption and Photoluminescence Properties. <i>Journal of Organic Chemistry</i> , 2019, 84, 15236-15254. | 1.7 | 13 |
| 12554 | Dynamic Polarizability and Higher-Order Electric Properties of Fluorene, Carbazole, and Dibenzofuran. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9753-9762. | 1.1 | 5 |
| 12555 | Host Prdx6 contributing to the intracellular survival of <i>Brucella suis</i> S2 strain. <i>BMC Veterinary Research</i> , 2019, 15, 304. | 0.7 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12556 | Investigating Differences and Similarities between Betaxolol Polymorphs. <i>Crystals</i> , 2019, 9, 509. | 1.0 | 7 |
| 12557 | A Mechanistic Study on the Tautomerism of H-Phosphonates, H-Phosphinates and Secondary Phosphine Oxides. <i>Molecules</i> , 2019, 24, 3859. | 1.7 | 24 |
| 12558 | Photostable Voltage-Sensitive Dyes Based on Simple, Solvatochromic, Asymmetric Thiazolothiazoles. <i>Journal of the American Chemical Society</i> , 2019, 141, 18780-18790. | 6.6 | 73 |
| 12559 | Use of the Phen ² NaDPO:Sn(SCN) ₂ Blend as Electron Transport Layer Results to Consistent Efficiency Improvements in Organic and Hybrid Perovskite Solar Cells. <i>Advanced Functional Materials</i> , 2019, 29, 1905810. | 7.8 | 41 |
| 12560 | Enantioselective Fluorocyclizations Mediated by Amino ² Acid ² -Derived Phthalazine. <i>Advanced Synthesis and Catalysis</i> , 2019, 361, 5334-5339. | 2.1 | 19 |
| 12561 | Synthesis and Catalytic Application of Kn ¹ lker-Type Iron Complexes with a Novel Asymmetric Cyclopentadienone Ligand Design. <i>Catalysts</i> , 2019, 9, 790. | 1.6 | 15 |
| 12562 | Sensitivity analysis of ship traffic in restricted two-way waterways considering the impact of LNG carriers. <i>Ocean Engineering</i> , 2019, 192, 106556. | 1.9 | 9 |
| 12563 | Interaction between water and carbon nanostructures: How good are current density functional approximations?. <i>Journal of Chemical Physics</i> , 2019, 151, 164702. | 1.2 | 47 |
| 12564 | Self ² -Assembly of Ferrocene Peptides: A Nonheme Strategy to Construct a Peroxidase Mimic. <i>Advanced Materials Interfaces</i> , 2019, 6, 1901082. | 1.9 | 10 |
| 12565 | Mechanomagnetics in Elastic Crystals: Insights from [Cu(acac) ₂]. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 15082-15088. | 7.2 | 36 |
| 12566 | Ex Vivo Analysis of Tryptophan Metabolism Using ¹⁹ F NMR. <i>ACS Chemical Biology</i> , 2019, 14, 1866-1873. | 1.6 | 5 |
| 12567 | Promoting a Significant Increase in the Photoluminescence Quantum Yield of Terbium(III) Complexes by Ligand Modification. <i>Inorganic Chemistry</i> , 2019, 58, 12099-12111. | 1.9 | 21 |
| 12568 | Myrmenaphthol A, Isolated from a Hawaiian Sponge of the Genus Myrmekioderma. <i>Journal of Natural Products</i> , 2019, 82, 2668-2671. | 1.5 | 4 |
| 12569 | Analyses on Molecular Properties of the Diamidinate Cr ^I -Cr ^I Complex by Multireference and DFT Approaches. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7803-7813. | 1.1 | 5 |
| 12570 | Covalent modification of phosphatidylethanolamine by 4-hydroxy-2-nonenal increases sodium permeability across phospholipid bilayer membranes. <i>Free Radical Biology and Medicine</i> , 2019, 143, 433-440. | 1.3 | 13 |
| 12571 | Performance Analysis and Optimization of Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) for Vertical Excitation Energies and Singlet ² -Triplet Energy Gaps. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7991-8000. | 1.1 | 27 |
| 12572 | Resonant inelastic X-ray scattering of a Ru photosensitizer: Insights from individual ligands to the electronic structure of the complete molecule. <i>Journal of Chemical Physics</i> , 2019, 151, 074701. | 1.2 | 12 |
| 12573 | Computational Investigation into the Ni(SeNHC ₂ (CN) ₂) ₂ and Ni(SNHC ₂ (CN) ₂) ₂ Complexes as Potential Catalysts for Hydrogen Production. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7822-7827. | 1.1 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12574 | Impact of molecular packing rearrangement on solid-state fluorescence: polyhalogenated <i>N</i> -hetarylamines vs. their co-crystals with 18-crown-6. <i>CrystEngComm</i> , 2019, 21, 5931-5946. | 1.3 | 12 |
| 12575 | Bonding and Diels-Alder reactions of substituted 2-borabicyclo(1.1.0)but-1(3)-enes: a theoretical study. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1. | 0.5 | 6 |
| 12576 | High-efficiency blue organic light-emitting Diodes using emissive carbazole-triazine-based donor-acceptor molecules with high reverse intersystem crossing rates. <i>Organic Electronics</i> , 2019, 75, 105399. | 1.4 | 6 |
| 12577 | Benzhydrylpyridinium Ions: A New Class of Thermometer Ions for the Characterization of Electrospray-Ionization Mass Spectrometers. <i>Analytical Chemistry</i> , 2019, 91, 11703-11711. | 3.2 | 23 |
| 12578 | A Bridging bis-Allyl Titanium Complex: Mechanistic Insights into the Electronic Structure and Reactivity. <i>Inorganic Chemistry</i> , 2019, 58, 12157-12166. | 1.9 | 4 |
| 12579 | Critical Evaluation of the Enthalpies of Formation for Fluorinated Compounds Using Experimental Data and High-Level Ab Initio Calculations. <i>Journal of Chemical & Engineering Data</i> , 2019, 64, 4863-4874. | 1.0 | 11 |
| 12580 | Insights into the Stability of Siloxy Carbene Intermediates and Their Corresponding Oxocarbenium Ions. <i>Journal of Organic Chemistry</i> , 2019, 84, 11813-11822. | 1.7 | 35 |
| 12581 | The synergy of different solid-state techniques to elucidate the supramolecular assembly of two 1-benzotriazole polymorphs. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19879-19889. | 1.3 | 4 |
| 12582 | Magnetic Feshbach resonances in ultracold collisions between Cs and Yb atoms. <i>Physical Review A</i> , 2019, 100, . | 1.0 | 12 |
| 12584 | Two Types of Hexanuclear Partial Tetracubane [Ni ₄ Ln ₂] (Ln = Dy, Tb, Ho) Complexes of Thioether-Based Schiff Base Ligands: Synthesis, Structure, and Comparison of Magnetic Properties. <i>Inorganic Chemistry</i> , 2019, 58, 12184-12198. | 1.9 | 37 |
| 12585 | Tetrakis(1,2,5-thiadiazolo)porphyrazines. 9. Synthesis and spectral and theoretical studies of the lithium(i) complex and its unusual behaviour in aprotic solvents in the presence of acids. <i>Dalton Transactions</i> , 2019, 48, 14049-14061. | 1.6 | 9 |
| 12586 | Carbazole-Appended Salen-Indium Conjugate Systems: Synthesis and Enhanced Luminescence Efficiency. <i>Inorganic Chemistry</i> , 2019, 58, 12358-12364. | 1.9 | 15 |
| 12587 | Sulfuric Acid Formation via H ₂ SO ₃ Oxidation by H ₂ O ₂ in the Atmosphere. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8385-8390. | 1.1 | 9 |
| 12588 | Hydroxyl Radical-Coupled Electron-Transfer Mechanism of Flavin-Dependent Hydroxylases. <i>Journal of Physical Chemistry B</i> , 2019, 123, 8065-8073. | 1.2 | 12 |
| 12589 | Revisiting π backbonding: the influence of d orbitals on metal-CO bonds and ligand red shifts. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20814-20821. | 1.3 | 26 |
| 12590 | Electron transfer in complexes of B ^{II} cations with organic π -acceptors: a combined experimental and quantum-chemical study. <i>Dalton Transactions</i> , 2019, 48, 14354-14366. | 1.6 | 4 |
| 12591 | Sulfamethoxazole degradation by an Fe(II)-activated persulfate process: insight into the reactive sites, product identification and degradation pathways. <i>Environmental Sciences: Processes and Impacts</i> , 2019, 21, 1560-1569. | 1.7 | 55 |
| 12592 | Synthesis, characterization, DFT study, DNA/BSA-binding affinity, and cytotoxicity of some dinuclear and trinuclear gold(III) complexes. <i>Journal of Biological Inorganic Chemistry</i> , 2019, 24, 1057-1076. | 1.1 | 19 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12593 | Amino-substituted naphthalene sulfonic acid/graphene composite as metal-free catalysts for oxygen reduction reactions. <i>Bulletin of the Chemical Society of Ethiopia</i> , 2019, 33, 359. | 0.5 | 4 |
| 12594 | Tuning of the Electro-Optical Properties of Tetraphenylcyclopentadienone via Substitution of Oxygen with Sterically-Hindered Electron Withdrawing Groups. <i>Scientific Reports</i> , 2019, 9, 12762. | 1.6 | 13 |
| 12595 | Structural evolution and electronic properties of Au ₂ Gen ⁿ⁺ /O (n=1~8) clusters: Anion photoelectron spectroscopy and theoretical calculations. <i>Chinese Journal of Chemical Physics</i> , 2019, 32, 229-240. | 0.6 | 9 |
| 12596 | Size effects in charge migration in alkyne chains. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1. | 0.5 | 9 |
| 12597 | Enhancement of Adhesion Strength of Perfluoroalkylpolyethers on Rough Glassy Silica for Antismudge Coatings. <i>ACS Applied Polymer Materials</i> , 2019, 1, 2613-2621. | 2.0 | 3 |
| 12598 | Diarylthiazole and diarylimidazole selective COX-1 inhibitor analysis through pharmacophore modeling, virtual screening, and DFT-based approaches. <i>Structural Chemistry</i> , 2019, 30, 2311-2326. | 1.0 | 17 |
| 12599 | pH-Controlled Chiral Packing and Self-Assembly of a Coumarin Tetrapeptide. <i>Langmuir</i> , 2019, 35, 12460-12468. | 1.6 | 17 |
| 12600 | Spin Crossover in Three Mononuclear Iron (III) Schiff Base Complexes. <i>Metals</i> , 2019, 9, 849. | 1.0 | 5 |
| 12601 | An Explanation about the Use of (S)-Citronellal as a Chiral Derivatizing Agent (CDA) in ¹ H and ¹³ C NMR for Sec-Butylamine, Methylbenzylamine, and Amphetamine: A Theoretical-Experimental Study. <i>Molecules</i> , 2019, 24, 2830. | 1.7 | 4 |
| 12602 | Theoretical insights into the stability of perovskite clusters by studying water adsorption on (CH ₃ NH ₃) ₄ SnI ₆ . <i>Solar Energy Materials and Solar Cells</i> , 2019, 202, 110126. | 3.0 | 3 |
| 12603 | AIRBED: A Simplified Density Functional Theory Model for Physisorption on Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5628-5634. | 2.3 | 8 |
| 12604 | DFT Studies on Metal-Controlled Regioselective Amination of <i>N</i> -Acylpyrazoles with Azodicarboxylates. <i>Journal of Organic Chemistry</i> , 2019, 84, 12399-12407. | 1.7 | 5 |
| 12605 | From Surface Hopping to Quantum Dynamics and Back. Finding Essential Electronic and Nuclear Degrees of Freedom and Optimal Surface Hopping Parameters. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8321-8332. | 1.1 | 24 |
| 12606 | Ligand's electronegativity controls the sense of enantioselectivity in BIFOP-X palladium-catalyzed allylic alkylations. <i>New Journal of Chemistry</i> , 2019, 43, 15743-15753. | 1.4 | 0 |
| 12607 | TiO ₂ @SrTiO ₃ Biphase Nanoceramics as Advanced Thermoelectric Materials. <i>Materials</i> , 2019, 12, 2895. | 1.3 | 11 |
| 12608 | A Reversible Phase Transition of 2D Coordination Layers by H ⁺ ™™™Cu(II) Interactions in a Coordination Polymer. <i>Molecules</i> , 2019, 24, 3204. | 1.7 | 7 |
| 12609 | Quantum mechanical static dipole polarizabilities in the QM7b and AlphaML showcase databases. <i>Scientific Data</i> , 2019, 6, 152. | 2.4 | 20 |
| 12610 | Synthesis of a copper-supported triplet nitrene complex pertinent to copper-catalyzed amination. <i>Science</i> , 2019, 365, 1138-1143. | 6.0 | 131 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12611 | Probing the Partial Activation of Water by Open-Shell Interactions, Cl(H ₂ O) ₄ . <i>Journal of Physical Chemistry A</i> , 2019, 123, 8657-8673. | 1.1 | 9 |
| 12612 | Machine Learning Protocol for Surface-Enhanced Raman Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6026-6031. | 2.1 | 60 |
| 12613 | Counterfeit and Substandard Test of the Antimalarial Tablet Riamet [®] by Means of Raman Hyperspectral Multicomponent Analysis. <i>Molecules</i> , 2019, 24, 3229. | 1.7 | 21 |
| 12614 | Electronic Structure, Vibrational Spectra, and Spin-Crossover Properties of Vacuum-Evaporable Iron(II) Bis(dihydrobis(pyrazolyl)borate) Complexes with Diimine Coligands. Origin of Giant Raman Features. <i>Inorganic Chemistry</i> , 2019, 58, 12873-12887. | 1.9 | 17 |
| 12615 | Structures, NMR Spectroscopic Features, and Cytotoxic Properties of Oligomeric Hellinoyl (<i>m</i>-GO-<i>m</i>-GOC)-Type Ellagitannins from the Galls of <i>Tamarix aphylla</i>. <i>Journal of Natural Products</i> , 2019, 82, 2682-2695. | 1.5 | 3 |
| 12616 | Chiral Phosphoric Acid-Catalyzed Enantioselective Direct Arylation of Iminoquinones: A Case Study of the Model Selectivity. <i>Journal of Organic Chemistry</i> , 2019, 84, 13473-13482. | 1.7 | 7 |
| 12617 | Extreme Scalability of DFT-Based QM/MM MD Simulations Using MiMiC. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5601-5613. | 2.3 | 32 |
| 12618 | Bio-inspired Molecular Redesign of a Multi-redox Catholyte for High-Energy Non-aqueous Organic Redox Flow Batteries. <i>CheM</i> , 2019, 5, 2642-2656. | 5.8 | 61 |
| 12619 | Inter-ligand delocalisations in transition metal complexes containing multiple non-innocent ligands. <i>Dalton Transactions</i> , 2019, 48, 14801-14807. | 1.6 | 7 |
| 12620 | Porous Ti/SnO ₂ -Sb anode as reactive electrochemical membrane for removing trace antiretroviral drug stavudine from wastewater. <i>Environment International</i> , 2019, 133, 105157. | 4.8 | 56 |
| 12621 | Ï-Extended Four-Coordinate Organoboron N,C-Chelates as Two-Photon Absorbing Chromophores. <i>Journal of Organic Chemistry</i> , 2019, 84, 13384-13393. | 1.7 | 11 |
| 12622 | Calculation of Free-Energy Barriers with TD-DFT: A Case Study on Excited-State Proton Transfer in Indigo. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8485-8495. | 1.1 | 16 |
| 12623 | Experimental and experimental-theoretical topological characteristics of the electron density distribution in the crystal of NCN-(2-pyridinecarbonitrile)-(3,6-di-tert-butylcatecholato)triphenylantimony(v). <i>Russian Chemical Bulletin</i> , 2019, 68, 1650-1655. | 0.4 | 7 |
| 12624 | Mechanistic Insight into the Ring-Opening Polymerization of É-Caprolactone and L-Lactide Using Ketiminate-Ligated Aluminum Catalysts. <i>Polymers</i> , 2019, 11, 1530. | 2.0 | 7 |
| 12625 | Group-transfer chemistry at transition metal centers in bulky alkoxide ligand environments. <i>Coordination Chemistry Reviews</i> , 2019, 400, 213044. | 9.5 | 12 |
| 12626 | Machine Learning in Computational Chemistry: An Evaluation of Method Performance for Nudged Elastic Band Calculations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6513-6523. | 2.3 | 19 |
| 12627 | Electrochemical Properties of N-Methyl- and N-Phenyl-2,4,6-Triphenylpyridium Perchlorate. <i>Russian Journal of Electrochemistry</i> , 2019, 55, 807-812. | 0.3 | 5 |
| 12628 | Structurally Diverse Covalent Triazine-Based Framework Materials for Photocatalytic Hydrogen Evolution from Water. <i>Chemistry of Materials</i> , 2019, 31, 8830-8838. | 3.2 | 111 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12629 | Revisiting the Potential Energy Surface of the Stacked Cytosine Dimer: FNO-CCSD(T) Interaction Energies, SAPT Decompositions, and Benchmarking. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9209-9222. | 1.1 | 9 |
| 12630 | A New Strategy of Design and Development of Aggregation-Induced Emission Materials Based on a Deep Insight into Mechanism. <i>Journal of Physical Chemistry C</i> , 2019, 123, 29379-29385. | 1.5 | 4 |
| 12631 | Detection of oxytetracycline in honey using SERS on silver nanoparticles. <i>TrAC - Trends in Analytical Chemistry</i> , 2019, 121, 115673. | 5.8 | 26 |
| 12632 | How Does Polymorphism Affect the Interfacial Charge-Transfer States in Organic Photovoltaics?. <i>Journal of Physical Chemistry C</i> , 2019, 123, 25585-25595. | 1.5 | 2 |
| 12633 | Bisaryl Diruthenium(III) Paddlewheel Complexes: Synthesis and Characterization. <i>Organometallics</i> , 2019, 38, 3888-3896. | 1.1 | 11 |
| 12634 | Prins cyclization of (-)-isopulegol with benzaldehyde for production of chromenols over organosulfonic clays. <i>Molecular Catalysis</i> , 2019, 478, 110569. | 1.0 | 7 |
| 12635 | Geometric and Electronic Structures of VB ₄ ^{0/+} Clusters and Reactivity of the Cationic Cluster with Methane from Quantum Chemical Calculations. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9223-9233. | 1.1 | 3 |
| 12636 | Electronic and Geometric Effects on Chemical Reactivity of 3d-Transition-Metal-Doped Silver Cluster Cations toward Oxygen Molecules. <i>Journal of Physical Chemistry C</i> , 2019, 123, 25890-25897. | 1.5 | 12 |
| 12637 | Nonprecious Catalyst for Three-Phase Contact in a Proton Exchange Membrane CO ₂ Conversion Full Cell for Efficient Electrochemical Reduction of Carbon Dioxide. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 40432-40442. | 4.0 | 10 |
| 12638 | Analytical energy gradient for the embedded cluster density approximation. <i>Journal of Chemical Physics</i> , 2019, 151, 134101. | 1.2 | 3 |
| 12639 | Crystal, Molecular, Electronic Structures and Spectroscopic Characteristics of N-Hydroxyamide of 3-[3,3-Dimethyl-1,2,3,4-Tetrahydroisoquinolin-1-iden]-2-Oxopropanoic Acid. <i>Journal of Structural Chemistry</i> , 2019, 60, 1396-1406. | 0.3 | 0 |
| 12640 | Spectral and quantum chemical analysis of ethyl 4-[3-(adamantan-1-yl)-4-phenyl-5-sulfanylidene-4,5-dihydro-1H-1,2,4-triazole-1-yl]methylpiperazine-1-carboxylate. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1950029. | 1.8 | 4 |
| 12641 | Complete cleavage of the N≡N triple bond by Ta ₂ N ₂ via degenerate ligand exchange at ambient temperature: A perfect catalytic cycle. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 21416-21420. | 3.3 | 60 |
| 12642 | A comparative study on cisplatin analogs containing 7-azaindole (7AIH) and its seven halogeno-derivatives: Vibrational spectra, DFT calculations and in vitro antiproliferative activity. Crystal and molecular structure of cis-[PtCl ₂ (4Br7AIH) ₂]-DMF. <i>Polyhedron</i> , 2019, 173, 114136. | 1.0 | 4 |
| 12643 | Preparation and characterization of benzotriazolium perrhenate. <i>Inorganica Chimica Acta</i> , 2019, 498, 119121. | 1.2 | 2 |
| 12644 | Measurement of the asymmetric UO ₂ ²⁺ stretching frequency for [UO ₂ (F) ₃]- using IRMPD spectroscopy. <i>International Journal of Mass Spectrometry</i> , 2019, 446, 116231. | 0.7 | 1 |
| 12645 | Growth and Characterization of Nonlinear Optical Crystal L-Isoleucine D-Norleucine: A DFT Approach. <i>Materials Today: Proceedings</i> , 2019, 8, 492-501. | 0.9 | 4 |
| 12646 | Photophysical, electrochemical, and DFT studies of the novel azacrown-bridged dinuclear ruthenium dye sensitizers for solar cells. <i>Polyhedron</i> , 2019, 173, 114106. | 1.0 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12647 | Solvation effect on binding modes of model lignin dimer compounds on MWW 2D-zeolite. <i>Journal of Chemical Physics</i> , 2019, 151, 114708. | 1.2 | 2 |
| 12648 | Facile synthesis of Pd(<i>ii</i>) and Ni(<i>ii</i>) pincer carbene complexes by the double C-H bond activation of a new hexahydropyrimidine-based bis(phosphine): catalysis of N couplings. <i>Dalton Transactions</i> , 2019, 48, 7203-7210. | 1.6 | 20 |
| 12649 | Comprehensive investigations on the action of cationic terthiophene and bithiophene as corrosion inhibitors: experimental and theoretical studies. <i>New Journal of Chemistry</i> , 2019, 43, 768-789. | 1.4 | 47 |
| 12650 | Exploiting the vicinal disubstituent effect on the diastereoselective synthesis of β^3 and $\hat{\Gamma}$ lactones. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 813-821. | 1.5 | 3 |
| 12651 | Deciphering the exceptional selectivity of semipinacol rearrangements in <i>cis</i> -fused $\hat{\Gamma}^2$ -lactam diols using high-level quantum chemical methods. <i>Organic Chemistry Frontiers</i> , 2019, 6, 725-731. | 2.3 | 5 |
| 12652 | Revealing quantum mechanical effects in enzyme catalysis with large-scale electronic structure simulation. <i>Reaction Chemistry and Engineering</i> , 2019, 4, 298-315. | 1.9 | 33 |
| 12653 | New copper(II) niflumate complexes with N-donor ligands: Synthesis, characterization and evaluation of anticancer potential against human cell lines. <i>Inorganica Chimica Acta</i> , 2019, 488, 260-268. | 1.2 | 18 |
| 12654 | A thermochemical computational study on hydroxyquinolines and their azulene analogues. <i>Journal of Molecular Structure</i> , 2019, 1183, 70-77. | 1.8 | 4 |
| 12655 | Insight into Compounds with Cu(H ₂ O) ₆ ²⁺ Units: New Ideas for Understanding Cu ²⁺ in Tutton Salts. <i>Journal of Physical Chemistry C</i> , 2019, 123, 3088-3101. | 1.5 | 19 |
| 12656 | Screened hybrid meta-GGA exchange correlation functionals for extended systems. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3002-3015. | 1.3 | 16 |
| 12657 | Probing enantioselectivity in rhodium-catalyzed Si-C bond cleavage to construct silicon-stereocenters: a theoretical study. <i>Catalysis Science and Technology</i> , 2019, 9, 646-651. | 2.1 | 8 |
| 12658 | Eco-friendly acetylcholine-carboxylate bio-ionic liquids for controllable N-methylation and N-formylation using ambient CO ₂ at low temperatures. <i>Green Chemistry</i> , 2019, 21, 567-577. | 4.6 | 68 |
| 12659 | Electrochemical properties of the [SiW ₁₀ O ₃₆ (M ₂ O ₂ E ₂) ₆] ⁿ⁻ polyoxometalate series (M = Mo(v) or W(v)); Tj ETQq0 0 0 rgBT /Overlock | 1.4 | 12 |
| 12660 | Investigation of cation binding and sensing by new crown ether core substituted naphthalene diimide systems. <i>New Journal of Chemistry</i> , 2019, 43, 2011-2018. | 1.4 | 11 |
| 12661 | Design considerations for chiral frustrated Lewis pairs: B/N FLPs derived from 3,5-bicyclic aryl piperidines. <i>Dalton Transactions</i> , 2019, 48, 133-141. | 1.6 | 7 |
| 12662 | Model potential study of non-valence correlation-bound anions of (C ₆₀) _n clusters: the role of electric field-induced charge transfer. <i>Faraday Discussions</i> , 2019, 217, 547-560. | 1.6 | 8 |
| 12663 | ¹ IL and ³ MLCT excited states modulated by H ⁺ : the structure and photophysical properties of [(2-bromo-5-(1 <i>H</i> -pyrazol-1-yl)pyrazine)Re(CO) ₃ Br]. <i>New Journal of Chemistry</i> , 2019, 43, 2449-2457. | 1.4 | 6 |
| 12664 | The effect of the second coordination sphere on the magnetism of [Ln(NO ₃) ₃ (H ₂ O) ₃] ⁺ (18-crown-6) (Ln = Dy and Er). <i>RSC Advances</i> , 2019, 9, 569-575. | 1.7 | 21 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12665 | Pushing the limits of concertedness. A waltz of wandering carbocations. <i>Chemical Science</i> , 2019, 10, 2159-2170. | 3.7 | 21 |
| 12666 | X-ray Raman optical activity of chiral molecules. <i>Chemical Science</i> , 2019, 10, 898-908. | 3.7 | 18 |
| 12667 | Halogen Bonding Interactions for Aromatic and Nonaromatic Explosive Detection. <i>ACS Sensors</i> , 2019, 4, 389-397. | 4.0 | 23 |
| 12668 | Anti-cancer organoruthenium(II) complexes and their interactions with cysteine and its analogues. A mass-spectrometric study. <i>Dalton Transactions</i> , 2019, 48, 2626-2634. | 1.6 | 20 |
| 12669 | Systematic Control of the Overlapping Energy Region for an Efficient Intramolecular Energy Transfer: Functionalized Salen Al /Triphenylamine Guest Host Assemblies. <i>Inorganic Chemistry</i> , 2019, 58, 2454-2462. | 1.9 | 13 |
| 12670 | Anion photoelectron spectroscopy of protein chromophores. <i>International Reviews in Physical Chemistry</i> , 2019, 38, 1-34. | 0.9 | 29 |
| 12671 | Calculation of $V_{S,\text{max}}$ and Its Use as a Descriptor for the Theoretical Calculation of pK_a Values for Carboxylic Acids. <i>Molecules</i> , 2019, 24, 79. | 1.7 | 13 |
| 12672 | The interaction of aluminum with catecholamine-based neurotransmitters: can the formation of these species be considered a potential risk factor for neurodegenerative diseases?. <i>Dalton Transactions</i> , 2019, 48, 6003-6018. | 1.6 | 16 |
| 12673 | Modulating the antitumoral activity by the design of new platinum(II) compounds: Synthesis, characterization, DFT, ultrastructure and mechanistic studies. <i>Journal of Inorganic Biochemistry</i> , 2019, 194, 200-213. | 1.5 | 8 |
| 12674 | Methoxy-substituted tetrakisquinoline analogs of EGTA and BAPTA for fluorescence detection of Cd^{2+} . <i>Dalton Transactions</i> , 2019, 48, 3840-3852. | 1.6 | 11 |
| 12675 | Assembly of T-Shaped Amphiphilic Thiazoles on the Air Water Interface: Impact of Polar Chromophore Moieties, as Well as Dipolarity and H -Extension of the Chromophore on the Supramolecular Structure. <i>Langmuir</i> , 2019, 35, 2587-2600. | 1.6 | 11 |
| 12676 | Desulfination versus decarboxylation as a means of generating three- and five-coordinate organopalladium complexes $[(\text{phen})_n\text{Pd}(\text{C}_6\text{H}_5)]^+$ ($n = 1$ and 2) to study their fundamental bimolecular reactivity. <i>Journal of Organometallic Chemistry</i> , 2019, 882, 42-49. | 0.8 | 6 |
| 12677 | High Efficiency Green InP Quantum Dot Based Electroluminescent Device Comprising Thick Shell Quantum Dots. <i>Advanced Optical Materials</i> , 2019, 7, 1801602. | 3.6 | 137 |
| 12678 | A Noncovalent Fluorescence Turn On Strategy for Hypoxia Imaging. <i>Angewandte Chemie</i> , 2019, 131, 2399-2403. | 1.6 | 24 |
| 12679 | Complexation of luteolin with lead (II): Spectroscopy characterization and theoretical researches. <i>Journal of Inorganic Biochemistry</i> , 2019, 193, 25-30. | 1.5 | 19 |
| 12680 | Remote Charge Effects on the Oxygen-Atom-Transfer Reactivity and Their Relationship to Molybdenum Enzymes. <i>Inorganic Chemistry</i> , 2019, 58, 2054-2068. | 1.9 | 14 |
| 12681 | Pyrazinoindole-Based Lewis-Acid/Base Assembly: Intriguing Intramolecular Charge-Transfer Switching through the Dual-Sensing of Fluoride and Acid. <i>Journal of Organic Chemistry</i> , 2019, 84, 3843-3852. | 1.7 | 8 |
| 12682 | Inhibition of T Cell Receptor Activation by Semi-Synthetic Sesquiterpene Lactone Derivatives and Molecular Modeling of Their Interaction with Glutathione and Tyrosine Kinase ZAP-70. <i>Molecules</i> , 2019, 24, 350. | 1.7 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12683 | A Noncovalent Fluorescence Turn-on Strategy for Hypoxia Imaging. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 2377-2381. | 7.2 | 123 |
| 12684 | A theoretical study on molecular structure, chemical reactivity and molecular docking studies on dalbergin and methylalbergin. <i>Journal of Molecular Structure</i> , 2019, 1183, 100-106. | 1.8 | 10 |
| 12685 | Rational Design of Reversible Molecular Photoswitches Based on Diarylethene Molecules. <i>Journal of Physical Chemistry C</i> , 2019, 123, 2736-2745. | 1.5 | 8 |
| 12686 | Direct evaluation of the force constant matrix in quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2019, 150, 034104. | 1.2 | 8 |
| 12687 | Predictable Substituent Control of CoIII/II Redox Potential and Spin Crossover in Bis(dipyridylpyrrolide)cobalt Complexes. <i>Inorganic Chemistry</i> , 2019, 58, 2218-2228. | 1.9 | 24 |
| 12688 | Host-Guest Interactions between Candesartan and Its Prodrug Candesartan Cilexetil in Complex with 2-Hydroxypropyl- β -cyclodextrin: On the Biological Potency for Angiotensin II Antagonism. <i>Molecular Pharmaceutics</i> , 2019, 16, 1255-1271. | 2.3 | 17 |
| 12689 | Studies on structure, NLO properties of a new organic NLO crystal: guanidinium 3,5-dihydroxybenzoate. <i>Journal of Materials Science: Materials in Electronics</i> , 2019, 30, 2994-3003. | 1.1 | 4 |
| 12690 | A Simple Model for Relative Energies of All Fullerenes Reveals the Interplay between Intrinsic Resonance and Structural Deformation Effects in Medium-Sized Fullerenes. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1255-1264. | 2.3 | 15 |
| 12691 | Revised M11 Exchange-Correlation Functional for Electronic Excitation Energies and Ground-State Properties. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2966-2990. | 1.1 | 76 |
| 12692 | Arylic versus Alkyl Hydrophobic Linkers Determine the Supramolecular Structure and Optoelectronic Properties of Tripodal Amphiphilic Push-Pull Thiazoles. <i>Langmuir</i> , 2019, 35, 2561-2570. | 1.6 | 17 |
| 12693 | The role of the dihedral angle and excited cation states in ionization and dissociation of mono-halogenated biphenyls; a combined experimental and theoretical coupled cluster study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4556-4567. | 1.3 | 4 |
| 12694 | Revealing the mechanism of contrasting charge transport properties for phenyl and thienyl substituent organic semiconductors. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4641-4649. | 1.3 | 5 |
| 12695 | Hydration Energies of Iron Hydroxide Cation: A Guided Ion Beam and Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1675-1688. | 1.1 | 2 |
| 12696 | Dioxygen Reduction to Hydrogen Peroxide by a Molecular Mn Complex: Mechanistic Divergence between Homogeneous and Heterogeneous Reductants. <i>Journal of the American Chemical Society</i> , 2019, 141, 4379-4387. | 6.6 | 51 |
| 12697 | Structural effect on the vapor-liquid equilibrium of toluene-ionic liquid systems. <i>Chemical Engineering Science</i> , 2019, 198, 1-15. | 1.9 | 27 |
| 12698 | A Ru(II)-p-cymene compound bearing naproxen-pyridineamide. Synthesis, spectroscopic studies, computational analysis and in vitro anticancer activity against lung cells compared to Ru(II)-p-cymene-naproxen and the corresponding drug ligands. <i>Inorganica Chimica Acta</i> , 2019, 489, 27-38. | 1.2 | 12 |
| 12699 | Corrected Structure of Natural Hyacinthacin C ₁ via Total Synthesis. <i>Journal of Natural Products</i> , 2019, 82, 358-367. | 1.5 | 10 |
| 12700 | Thermoresponsive Graphene Membranes with Reversible Gating Regularity for Smart Fluid Control. <i>Advanced Functional Materials</i> , 2019, 29, 1808501. | 7.8 | 70 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12701 | A cascade mechanism for a simple reaction: The gas-phase methylation of phenol with methanol. <i>Journal of Catalysis</i> , 2019, 370, 447-460. | 3.1 | 23 |
| 12702 | The effect of 2-, 3- and 4-pyridyl substituents on photophysics of fac-[ReCl(CO) ₃ (n-pytpy- $\hat{\text{I}}^{\text{2N}}$)] complexes: Experimental and theoretical insights. <i>Journal of Luminescence</i> , 2019, 209, 346-356. | 1.5 | 8 |
| 12703 | Influence of acceptors in NLOphoric acenaphthene and morpholine-thiourea hybrid dyes: Photophysical, viscosity, DFT and Z-Scan study. <i>Optical Materials</i> , 2019, 89, 178-190. | 1.7 | 7 |
| 12704 | Exploiting the Aromatic Chameleon Character of Fulvenes for Computational Design of Baird's Aromatic Triplet Ground State Compounds. <i>Chemistry - an Asian Journal</i> , 2019, 14, 1870-1878. | 1.7 | 13 |
| 12705 | <i>De novo</i> prediction of cross-effect efficiency for magic angle spinning dynamic nuclear polarization. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2166-2176. | 1.3 | 32 |
| 12706 | Effect of hydrogen bonding on innocent and non-innocent axial ligands bound to iron porphyrins. <i>Dalton Transactions</i> , 2019, 48, 7179-7186. | 1.6 | 14 |
| 12707 | Electronic spectra of ions of astrochemical interest: from fast overview spectra to high resolution. <i>Faraday Discussions</i> , 2019, 217, 98-113. | 1.6 | 12 |
| 12708 | Synthesis and electronic properties of A ₃ B-thienyl porphyrins: experimental and computational investigations. <i>New Journal of Chemistry</i> , 2019, 43, 1569-1580. | 1.4 | 20 |
| 12709 | Effects of pore surfaces on the electronic states of metal complexes formed on bipyridine periodic mesoporous organosilica. <i>New Journal of Chemistry</i> , 2019, 43, 2471-2478. | 1.4 | 6 |
| 12710 | A dipole-dipole interaction tuning the photoluminescence of silicon quantum dots in a water vapor environment. <i>Nanoscale</i> , 2019, 11, 1790-1797. | 2.8 | 4 |
| 12711 | A colorless semi-aromatic polyimide derived from a sterically hindered bromine-substituted dianhydride exhibiting dual fluorescence and phosphorescence emission. <i>Materials Chemistry Frontiers</i> , 2019, 3, 39-49. | 3.2 | 38 |
| 12712 | A tunable positive and negative photoconductive photodetector based on a gold/graphene/p-type silicon heterojunction. <i>Journal of Materials Chemistry C</i> , 2019, 7, 887-896. | 2.7 | 32 |
| 12713 | Spectrophotometric and RGB performances of a new tetraphenylcyclopenta-derived Schiff base for the quantification of cyanide ions. <i>Analytical Methods</i> , 2019, 11, 1137-1143. | 1.3 | 29 |
| 12714 | Aggregation-caused quenching <i>versus</i> crystallization induced emission in thiazolo[5,4- <i>b</i>]thieno[3,2- <i>e</i>]pyridine (TTP) derivatives: theoretical insights. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 46-56. | 1.3 | 39 |
| 12715 | Probing the gas-phase structure of charge-tagged intermediates of a proline catalyzed aldol reaction - vibrational spectroscopy distinguishes oxazolidinone from enamine species. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2578-2586. | 1.3 | 0 |
| 12716 | Photochemistry of dithiophosphate Ni(S ₂ P(i-Bu) ₂) ₂ complex in CCl ₄ . Transient species and TD-DFT calculations. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 381, 111857. | 2.0 | 3 |
| 12717 | Exploring Hydrogen Evolution Accompanying Nitrogen Reduction on Biomimetic Nitrogenase Analogs: Can Fe-NxHy Intermediates Be Active Under Turnover Conditions?. <i>Inorganic Chemistry</i> , 2019, 58, 7969-7977. | 1.9 | 8 |
| 12718 | Energetics of exciton binding and dissociation in polythiophenes: a tight binding approach. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 11999-12011. | 1.3 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12719 | Reassessment of the Mechanisms of Thermal C-H Bond Activation of Methane by Cationic Magnesium Oxides: A Critical Evaluation of the Suitability of Different Density Functionals. <i>ChemPhysChem</i> , 2019, 20, 1812-1821. | 1.0 | 5 |
| 12720 | Influence of Sulfur Oxidation State and Substituents on Sulfur-Bridged Luminescent Copper(I) Complexes Showing Thermally Activated Delayed Fluorescence. <i>Inorganic Chemistry</i> , 2019, 58, 7156-7168. | 1.9 | 31 |
| 12721 | Betulin-1,4-quinone hybrids: Synthesis, anticancer activity and molecular docking study with NQO1 enzyme. <i>European Journal of Medicinal Chemistry</i> , 2019, 177, 302-315. | 2.6 | 27 |
| 12722 | Modification of a Carbon Nanobelt with Actinides ThAm: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4900-4907. | 1.1 | 3 |
| 12723 | Alkali carbonates promote CO ₂ capture by sodium orthosilicate. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13135-13143. | 1.3 | 20 |
| 12724 | Silicanes Modified by Conjugated Substituents for Optoelectronic Devices. <i>Advanced Optical Materials</i> , 2019, 7, 1900696. | 3.6 | 8 |
| 12725 | Dihydrogen Splitting by Intramolecular Borane-Phosphane Frustrated Lewis Pairs: A Comprehensive Characterization Strategy Using Solid State NMR and DFT Calculations. <i>ChemPhysChem</i> , 2019, 20, 1837-1849. | 1.0 | 5 |
| 12726 | P/N co-doped carbon derived from cellulose: A metal-free photothermal catalyst for transfer hydrogenation of nitroarenes. <i>Applied Surface Science</i> , 2019, 487, 616-624. | 3.1 | 22 |
| 12727 | Synthesis, crystal structure, spectroscopic characterization and nonlinear optical properties of (Z)-N'-(2,4-dinitrobenzylidene)-2-(quinolin-8-yloxy) acetohydrazide. <i>Journal of Molecular Structure</i> , 2019, 1194, 112-123. | 1.8 | 50 |
| 12728 | Proton Abstraction from DME _n ·X ⁺ by OH ⁻ , O ₂ ⁻ , and XO ₂ ⁻ , for X = Li, Na, and K: Implications for Li-O ₂ Batteries. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4942-4947. | 1.1 | 4 |
| 12729 | Theoretical Insights Into the Depolymerization Mechanism of Lignin to Methyl p-hydroxycinnamate by [Bmim][FeCl ₄] Ionic Liquid. <i>Frontiers in Chemistry</i> , 2019, 7, 446. | 1.8 | 14 |
| 12730 | Di-manganese(0) carbonyl mediated azo bond cleavage and recombination reaction in azo-aromatic ligand: An effect of extended phenolate donor. <i>Polyhedron</i> , 2019, 172, 182-190. | 1.0 | 0 |
| 12731 | Facile Access to Challenging <i>ortho</i> -Terphenyls via Merging Two Multi-Step Domino Reactions in One-Pot: A Joint Experimental/Theoretical Study. <i>ChemCatChem</i> , 2019, 11, 3982-3992. | 1.8 | 8 |
| 12732 | QM/MM Calculations for the Cl ⁻ + CH ₃ Cl S _N 2 Reaction in Water Using CM5 Charges and Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5713-5717. | 1.1 | 11 |
| 12733 | Synthesis and anticancer activity novel dimeric azatriperoxides. <i>RSC Advances</i> , 2019, 9, 18923-18929. | 1.7 | 22 |
| 12734 | The solid-state structure of the β -blocker metoprolol: a combined experimental and <i>in silico</i> investigation. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 87-96. | 0.2 | 12 |
| 12735 | In silico structure-based design of GABA B receptor agonists using a combination of docking and QSAR. <i>Chemical Biology and Drug Design</i> , 2019, 94, 1782-1798. | 1.5 | 7 |
| 12736 | Introducing a Nonvolatile N-type Dopant Drastically Improves Electron Transport in Polymer and Small-Molecule Organic Transistors. <i>Advanced Functional Materials</i> , 2019, 29, 1902784. | 7.8 | 35 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12737 | Structural and Electronic Properties of Oxidized and Amorphous Nanodiamond Surfaces with Covalently Grafted Polypyrrole. <i>Physica Status Solidi (B): Basic Research</i> , 2019, 256, 1900176. | 0.7 | 2 |
| 12738 | Hybrid QSPR models for the prediction of the free energy of solvation of organic solute/solvent pairs. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13706-13720. | 1.3 | 33 |
| 12739 | Triarylborane-Based Helical Donor-Acceptor Compounds: Synthesis, Photophysical, and Electronic Properties. <i>Chemistry - A European Journal</i> , 2019, 25, 10845-10857. | 1.7 | 27 |
| 12740 | Diphospho-Ureas from the Phosphaketene Ph ₃ GePCO. <i>Chemistry - A European Journal</i> , 2019, 25, 10084-10087. | 1.7 | 10 |
| 12741 | Influence of Coulombic Interaction on the Interfacial Self-Assembly of Discotic Liquid Crystal Amphiphiles: A Combined Experimental and Computer Simulation Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16681-16689. | 1.5 | 4 |
| 12742 | Direct synthesis of furfuryl alcohol from furfural: catalytic performance of monometallic and bimetallic Mo and Ru phosphides. <i>Catalysis Science and Technology</i> , 2019, 9, 3656-3668. | 2.1 | 35 |
| 12743 | Modeling L _{2,3} -edge X-ray absorption spectroscopy with linear response exact two-component relativistic time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2019, 150, 234103. | 1.2 | 28 |
| 12744 | Nuclear dynamics in resonant inelastic X-ray scattering and X-ray absorption of methanol. <i>Journal of Chemical Physics</i> , 2019, 150, 234301. | 1.2 | 26 |
| 12745 | Calculation of scalar nuclear spin-spin coupling in a noble-gas mixture. <i>Physical Review A</i> , 2019, 99, . | 1.0 | 8 |
| 12746 | Synthesis, Structure, and Catalytic Reactivity of Pd(II) Complexes of Proline and Proline Homologs. <i>Catalysts</i> , 2019, 9, 515. | 1.6 | 7 |
| 12747 | How does the pH influences the Ru-NO coordination compounds?. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25999. | 1.0 | 2 |
| 12748 | An ab initio study of the valence tautomerism of type B mesoionic rings. <i>Tetrahedron Letters</i> , 2019, 60, 150876. | 0.7 | 7 |
| 12749 | Direct Chemical Synthesis of Benzyl-Modified Silicane from Calcium Disilicide. <i>Chemistry of Materials</i> , 2019, 31, 4720-4725. | 3.2 | 16 |
| 12750 | Dynamic Behavior of C ₆₀ Fullerene in Carbon Nanopeapods: Tight-Binding Molecular Dynamics Simulation. <i>Bulletin of the Korean Chemical Society</i> , 2019, 40, 724-728. | 1.0 | 5 |
| 12751 | Solid state NMR and computational studies on cyclopentadienyl lithium. <i>Journal of Molecular Modeling</i> , 2019, 25, 196. | 0.8 | 2 |
| 12752 | Excited State Dynamics of Isocyano Rhenium(I) Phenanthroline Complexes from Time-Resolved Spectroscopy. <i>ChemPhysChem</i> , 2019, 20, 1946-1953. | 1.0 | 8 |
| 12753 | Structural and magnetic characterization of Ni(ⁱⁱ), Co(ⁱⁱ), and Fe(ⁱⁱ) binuclear complexes on a bis(pyridyl-triazolyl)alkane basis. <i>Dalton Transactions</i> , 2019, 48, 10526-10536. | 1.6 | 6 |
| 12754 | Geometry, stability and aromaticity of \hat{I}^2 -diketiminato-coordinated alkaline-earth compounds. <i>Chinese Chemical Letters</i> , 2019, 30, 2249-2253. | 4.8 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12755 | Computational study on the catalyst-controlled synthesis of C2-substituted quinolines through the annulation of 2-vinylanilines and alkynoates. <i>Journal of Organometallic Chemistry</i> , 2019, 897, 7-12. | 0.8 | 0 |
| 12756 | Extracting Design Principles for Efficient Thermally Activated Delayed Fluorescence (TADF) from a Simple Four-State Model. <i>Chemistry of Materials</i> , 2019, 31, 6995-7006. | 3.2 | 84 |
| 12757 | Synthesis, photophysical and electronic properties of tetra-donor- or acceptor-substituted <i>ortho</i> -perylene displaying four reversible oxidations or reductions. <i>Chemical Science</i> , 2019, 10, 7516-7534. | 3.7 | 45 |
| 12758 | Predictive chirality sensing via Schiff base formation. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 6699-6705. | 1.5 | 6 |
| 12759 | A computational investigation on the electronic and optical properties of Coronene and its Boron-Nitride and perfluorinated counterparts. <i>Journal of Physics: Conference Series</i> , 2019, 1226, 012016. | 0.3 | 3 |
| 12760 | From 3D to 2D Transition Metal Nitroprussides by Selective Rupture of Axial Bonds. <i>Chemistry - A European Journal</i> , 2019, 25, 11327-11336. | 1.7 | 22 |
| 12761 | Structural Elucidation of Presilphiperfolane-7 β ,8 β -diol, a Bioactive Sesquiterpenoid from <i>Pulicaria vulgaris</i> : A Combined Approach of Solvent-Induced Chemical Shifts, GIAO Calculation of Chemical Shifts, and Full Spin Analysis. <i>Journal of Natural Products</i> , 2019, 82, 1874-1885. | 1.5 | 23 |
| 12762 | The CUAGAU Set of Coupled-Cluster Reference Data for Small Copper, Silver, and Gold Compounds and Assessment of DFT Methods. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5781-5788. | 1.1 | 24 |
| 12763 | Theoretical Approaches for Modeling the Effect of the Electrode Potential in the SERS Vibrational Wavenumbers of Pyridine Adsorbed on a Charged Silver Surface. <i>Frontiers in Chemistry</i> , 2019, 7, 423. | 1.8 | 13 |
| 12764 | Prediction of emission wavelengths of phosphorescent NHC based emitters for OLEDs. <i>Tetrahedron</i> , 2019, 75, 130431. | 1.0 | 3 |
| 12765 | Mapping free energy regimes in electrocatalytic reductions to screen transition metal-based catalysts. <i>Chemical Science</i> , 2019, 10, 7649-7658. | 3.7 | 6 |
| 12766 | Double- and multi-slit interference in photodetachment from nanometer organic molecular anions. <i>Journal of Chemical Physics</i> , 2019, 150, 244302. | 1.2 | 0 |
| 12767 | Electronically Nonadiabatic Structural Transformations Promoted by Electron Beams. <i>Advanced Functional Materials</i> , 2019, 29, 1901901. | 7.8 | 12 |
| 12768 | A computational study on the redox properties and binding affinities of iron complexes of hydroxypyridinones. <i>Journal of Molecular Modeling</i> , 2019, 25, 172. | 0.8 | 4 |
| 12769 | Monodispersed CuSe Sensitized Covalent Organic Framework Photosensitizer with an Enhanced Photodynamic and Photothermal Effect for Cancer Therapy. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 23072-23082. | 4.0 | 117 |
| 12770 | Mesoionic 1,2,3-triazolo[1,5-a]pyridine β -ylidenes in Phosphorescent Platinum(II) Complexes. <i>ChemPhotoChem</i> , 2019, 3, 1000-1003. | 1.5 | 6 |
| 12771 | Investigation of molecular structure and solvent/temperature effect on tautomerism in (E)-4,6-dibromo-3-methoxy-2-[(p-tolylimino)methyl]phenol, a new thermochromic Schiff base, by using XRD, FT-IR, UV-vis, NMR and DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 222, 117198. | 2.0 | 11 |
| 12772 | Preparation of Size- and Composition-Controlled Pt _n Sn _x /SiO ₂ (n = 4, 7, 24) Bimetallic Model Catalysts with Atomic Layer Deposition. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16194-16209. | 1.5 | 25 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12773 | A study of UV-vis spectroscopic and DFT calculation of the UV absorber in different solvent. <i>Progress in Organic Coatings</i> , 2019, 135, 168-175. | 1.9 | 9 |
| 12774 | Observation of an Inversion in Photophysical Tuning in a Systematic Study of Luminescent Triazole-Based Osmium(II) Complexes. <i>Inorganic Chemistry</i> , 2019, 58, 8607-8621. | 1.9 | 5 |
| 12775 | Mechanistic investigation-inspired activation mode of DBU and the function of the $\hat{\iota}$ -diazo group in the reaction of the $\hat{\iota}$ -amino ketone compound and EDA: [DBU-H] ⁺ -DMF-H ₂ O and $\hat{\iota}$ -diazo as strong N-terminal nucleophiles. <i>Organic Chemistry Frontiers</i> , 2019, 6, 2678-2686. | 2.3 | 2 |
| 12776 | DFT Investigation of Graphene Nanoribbon As a Potential Nanobiosensor for Tyrosine Amino Acid. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 778-785. | 0.1 | 18 |
| 12777 | [Cp ₂ Mo(OH)(OH ₂)] ⁺ -Catalyzed Hydrolysis of Mono- and Difunctional Ethers: Theoretical Understanding of Their Divergent Reactivity. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 2924-2932. | 1.0 | 1 |
| 12778 | Ab initio kinetics for pyrolysis and combustion systems. <i>Computer Aided Chemical Engineering</i> , 2019, , 115-167. | 0.3 | 27 |
| 12779 | Designed self-assembly of iron encapsulated doped porous carbon as durable electrocatalyst for oxygen reduction reaction in alkaline medium. <i>Carbon</i> , 2019, 152, 616-630. | 5.4 | 5 |
| 12780 | Selective leaching of Al from hypereutectic Al-Si alloy to produce nano-porous silicon (NPS) anodes for lithium ion batteries. <i>Electrochimica Acta</i> , 2019, 317, 654-662. | 2.6 | 34 |
| 12781 | Studies of Redox Cofactor Pyrroloquinoline Quinone and Its Interaction with Lanthanides(III) and Calcium(II). <i>Inorganic Chemistry</i> , 2019, 58, 8432-8441. | 1.9 | 27 |
| 12782 | Covalency and magnetic anisotropy in lanthanide single molecule magnets: the DyDOTA archetype. <i>Chemical Science</i> , 2019, 10, 7233-7245. | 3.7 | 64 |
| 12783 | Disentangling Electronic and Vibrational Effects in the Prediction of Band Shapes for Singlet-Triplet Transitions. <i>Journal of Physical Chemistry C</i> , 2019, 123, 14173-14179. | 1.5 | 10 |
| 12784 | Using Density Functional Theory Based Methods to Investigate the Photophysics of Polycyclic Aromatic Hydrocarbon Radical Cations: A Benchmark Study on Naphthalene, Pyrene and Perylene Cations. <i>ChemPhotoChem</i> , 2019, 3, 763-769. | 1.5 | 6 |
| 12785 | Thermochemistry of phosphorus sulfide cages: an extreme challenge for high-level ab initio methods. <i>Structural Chemistry</i> , 2019, 30, 1665-1675. | 1.0 | 4 |
| 12786 | Minimally Empirical Double-Hybrid Functionals Trained against the GMTKN55 Database: revDSD-PBEP86-D4, revDOD-PBE-D4, and DOD-SCAN-D4. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5129-5143. | 1.1 | 262 |
| 12787 | Electrophilic Aromatic Substitution Reactions: Mechanistic Landscape, Electrostatic and Electric-Field Control of Reaction Rates, and Mechanistic Crossovers. <i>Journal of the American Chemical Society</i> , 2019, 141, 9719-9730. | 6.6 | 62 |
| 12788 | A theoretical analysis of the structure and properties of B ₂₆ H ₃₀ isomers. Consequences to the laser and semiconductor doping capabilities of large borane clusters. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12916-12923. | 1.3 | 5 |
| 12789 | Molecular rearrangements of poststerone derivative steroid core with formation of unique D-homostructures of pregnane and androstane series. <i>Steroids</i> , 2019, 148, 28-35. | 0.8 | 4 |
| 12790 | Twelve Cadmium(II) Coordination Frameworks with Asymmetric Pyridinyl Triazole Carboxylate: Syntheses, Structures, and Fluorescence Properties. <i>Crystal Growth and Design</i> , 2019, 19, 3785-3806. | 1.4 | 41 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12791 | Adsorption/Absorption of Lithium Affecting the Growth Morphology of Aragonite. The Two-Dimensional Epitaxy of Li_2CO_3 (Zabuyelite) on the {001} Form of Aragonite (CaCO_3). <i>Crystal Growth and Design</i> , 2019, 19, 3969-3978. | 1.4 | 4 |
| 12792 | Intriguing Effects of Halogen Substitution on the Photophysical Properties of 2,9-(Bis)halo-Substituted Phenanthrolinecopper(I) Complexes. <i>Inorganic Chemistry</i> , 2019, 58, 7730-7745. | 1.9 | 23 |
| 12793 | The optimal DFT approach in DP4 NMR structure analysis – pushing the limits of relative configuration elucidation. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 5886-5890. | 1.5 | 41 |
| 12794 | Productive reorientation of a bound oxime reactivator revealed in room temperature X-ray structures of native and VX-inhibited human acetylcholinesterase. <i>Journal of Biological Chemistry</i> , 2019, 294, 10607-10618. | 1.6 | 13 |
| 12795 | Assessment of DFT Methods for Transition Metals with the TMC151 Compilation of Data Sets and Comparison with Accuracies for Main-Group Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3610-3622. | 2.3 | 85 |
| 12796 | DFT perspective on the selectivity and mechanism of ligand-free Heck reaction involving allylic esters and arenediazonium salts. <i>Journal of Organometallic Chemistry</i> , 2019, 896, 5-15. | 0.8 | 10 |
| 12797 | Naphthoquinone derivative-based dye for dye-sensitized solar cells: experimental and computational aspects. <i>Materials Research Express</i> , 2019, 6, 085537. | 0.8 | 15 |
| 12798 | Synergy between Ionic Liquids and CuCl_2 in Gas-Liquid Phase Reactions of Acetylene Hydrochlorination. <i>Catalysts</i> , 2019, 9, 504. | 1.6 | 13 |
| 12799 | Selenium-linked liquid crystal dimers for twist-bend nematogens. <i>Journal of Molecular Liquids</i> , 2019, 289, 111097. | 2.3 | 28 |
| 12800 | Mechanistic Study on the Asymmetric Synthesis of the Wieland-Miescher Ketone and Analogs. <i>ChemCatChem</i> , 2019, 11, 4064-4071. | 1.8 | 5 |
| 12801 | Yeast cell wall – Silver nanoparticles interaction: A synergistic approach between surface-enhanced Raman scattering and computational spectroscopy tools. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 222, 117223. | 2.0 | 15 |
| 12802 | Enhancing the supramolecular stability of monolayers by combining dipolar with amphiphilic motifs: a case of amphiphilic push-pull-thiazole. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13241-13247. | 1.3 | 7 |
| 12803 | An Experimental and Theoretical Investigation of 1-Butanol Pyrolysis. <i>Frontiers in Chemistry</i> , 2019, 7, 326. | 1.8 | 12 |
| 12804 | Computational prediction of chiroptical properties in structure elucidation of natural products. <i>Natural Product Reports</i> , 2019, 36, 1005-1030. | 5.2 | 66 |
| 12805 | ss-NMR and single-crystal X-ray diffraction in the elucidation of a new polymorph of bischalcone (1 <i>E</i> ,4 <i>E</i>)-1,5-bis(4-fluorophenyl)penta-1,4-dien-3-one. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 694-701. | 0.2 | 2 |
| 12806 | The quest for a triplet ground-state alkene: Highly twisted C=C double bonds. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3965. | 0.9 | 7 |
| 12807 | Substituent effects on the aromaticity of benzene – An approach based on interaction coordinates. <i>Journal of Chemical Physics</i> , 2019, 150, 214108. | 1.2 | 8 |
| 12808 | Polynuclear Glycinehydroximate Cu(II)–Gd(III) Metallamacrocyclic Complexes: Halochromic Properties. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2019, 45, 356-360. | 0.3 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12809 | Prediction of Excited-State Properties of Oligoacene Crystals Using Fragment-Based Quantum Mechanical Method. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5407-5417. | 1.1 | 18 |
| 12810 | Early impairment of epigenetic pattern in neurodegeneration: Additional mechanisms behind pyrethroid toxicity. <i>Experimental Gerontology</i> , 2019, 124, 110629. | 1.2 | 27 |
| 12811 | Photophysical processes for phenanthroline-menthol ligand and its Eu(III) and Tb(III) complexes in solution. <i>Journal of Luminescence</i> , 2019, 214, 116548. | 1.5 | 0 |
| 12812 | Halogen-substituent effect on the spectroscopic properties of 2-phenyl-6-dimethylaminobenzothiazoles. <i>Tetrahedron Letters</i> , 2019, 60, 1702-1705. | 0.7 | 3 |
| 12813 | Influence of N-Substitution on the Formation and Oxidation of NHC-CAAC-Derived Triazaalkenes. <i>Journal of Organic Chemistry</i> , 2019, 84, 8899-8909. | 1.7 | 17 |
| 12814 | Rotational barriers of carbamate-protected amine crosslinkers for hydrogels: A combined experimental and computational study. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3936. | 0.9 | 4 |
| 12815 | Synthesis of polyaminophosphonic acid-functionalized poly(glycidyl methacrylate) for the efficient sorption of La(III) and Y(III). <i>Chemical Engineering Journal</i> , 2019, 375, 121932. | 6.6 | 46 |
| 12816 | Suppressing the Shuttle Effect in Lithium-Sulfur Batteries by a UiO-66-Modified Polypropylene Separator. <i>ACS Omega</i> , 2019, 4, 10328-10335. | 1.6 | 57 |
| 12817 | Quantum Mechanical Modeling of the Vibrational Spectra of Minerals with a Focus on Clays. <i>Minerals (Basel, Switzerland)</i> , 2019, 9, 141. | 0.8 | 18 |
| 12818 | Cationic dyes adsorption by Na-Montmorillonite Nano Clay: Experimental study combined with a theoretical investigation using DFT-based descriptors and molecular dynamics simulations. <i>Journal of Molecular Liquids</i> , 2019, 290, 111139. | 2.3 | 103 |
| 12819 | Theoretical Search for the Highest Valence States of the Coinage Metals: Roentgenium Heptafluoride May Exist. <i>Inorganic Chemistry</i> , 2019, 58, 8735-8738. | 1.9 | 4 |
| 12820 | A Fast Transient Absorption Study of Co(AcAc) ₃ . <i>Frontiers in Chemistry</i> , 2019, 7, 348. | 1.8 | 5 |
| 12821 | Modulating absorption and charge transfer in bodipy-carbazole donor-acceptor dyads through molecular design. <i>Dalton Transactions</i> , 2019, 48, 8488-8501. | 1.6 | 20 |
| 12822 | Quantum chemical calculations for the norbadione A complexes with Cs ⁺ , K ⁺ , and Na ⁺ in gas and aqueous phases. <i>Chemical Physics Letters</i> , 2019, 730, 26-31. | 1.2 | 2 |
| 12823 | Bacterial Tetrabromopyrrole Debrominase Shares a Reductive Dehalogenation Strategy with Human Thyroid Deiodinase. <i>Biochemistry</i> , 2019, 58, 5329-5338. | 1.2 | 13 |
| 12824 | A Series of Quinolinol-Based Indium Luminophores: A Rational Design Approach for Manipulating Photophysical Properties. <i>Inorganic Chemistry</i> , 2019, 58, 8056-8063. | 1.9 | 8 |
| 12825 | Mixtures of LiTFSI and urea: ideal thermodynamic behavior as key to the formation of deep eutectic solvents?. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12279-12287. | 1.3 | 20 |
| 12826 | Cyclometalated Platinum(II) Complexes with Mesoionic Dibenzofuranyl-1,2,3-triazol-4-ylidene Ligands: Synthesis, Characterization and Photophysical Properties. <i>ChemPhotoChem</i> , 2019, 3, 554-558. | 1.5 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 12827 | New global minima of 6-vertex dicarboranes: classical but unexpected. <i>Chemical Communications</i> , 2019, 55, 6373-6376. | 2.2 | 4 |
| 12828 | Topological analysis of CeMn ₅ (M ²⁺ =Co, Rh) electron charge densities. <i>Computational Materials Science</i> , 2019, 164, 205-217. | 1.4 | 3 |
| 12829 | Axial ligand mediated switchable rotary motions in a ferrocene-bridged diiron(III) porphyrin dimer. <i>Journal of Organometallic Chemistry</i> , 2019, 894, 28-38. | 0.8 | 14 |
| 12830 | UV-Vis Absorption Spectroscopy of Polonium(IV) Chloride Complexes: An Electronic Structure Theory Study. <i>Inorganic Chemistry</i> , 2019, 58, 7036-7043. | 1.9 | 6 |
| 12831 | Palladium/XuPhos-Catalyzed Enantioselective Carbiodination of Olefin-Tethered Aryl Iodides. <i>Journal of the American Chemical Society</i> , 2019, 141, 8110-8115. | 6.6 | 135 |
| 12832 | The effect of locking π -conjugation in organoboron moieties in the structures of luminescent tetracoordinate boron complexes. <i>Dalton Transactions</i> , 2019, 48, 8642-8663. | 1.6 | 24 |
| 12833 | A general study of actinyl hydration by molecular dynamics simulations using <i>ab initio</i> force fields. <i>Journal of Chemical Physics</i> , 2019, 150, 104504. | 1.2 | 13 |
| 12834 | Formation of two centre three electron bond by hydroxyl radical induced reaction of thiocoumarin: evidence from experimental and theoretical studies. <i>Free Radical Research</i> , 2019, 53, 629-640. | 1.5 | 7 |
| 12835 | Addition of the Lewis Acid Zn(C ₆ F ₅) ₂ Enables Organic Transistors with a Maximum Hole Mobility in Excess of 20 cm ² V ⁻¹ s ⁻¹ . <i>Advanced Materials</i> , 2019, 31, e1900871. | 11.1 | 64 |
| 12836 | Nature of interlayer carbon-carbon covalent bonding in graphene-based materials. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1. | 0.5 | 5 |
| 12837 | Electronic and optical properties of sulfur and nitrogen doped graphene quantum dots: A theoretical study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019, 113, 130-136. | 1.3 | 28 |
| 12838 | Rational Design of 5-(4-(Isopropylsulfonyl)phenyl)-3-(3-(4-((methylamino)methyl)phenyl)isoxazol-5-yl)pyrazin-2-amine (VX-970, M6620): Optimization of Intra- and Intermolecular Polar Interactions of a New Ataxia Telangiectasia Mutated and Rad3-Related (ATR) Kinase Inhibitor. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 5547-5561. | 2.9 | 34 |
| 12839 | Host-Guest Complexes of Dodeka(ethylene)octamine: Prediction of Ion Selectivity by Quantum Chemical Calculations IX. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2019, 645, 701-705. | 0.6 | 7 |
| 12840 | A DFT Study of the Modulation of the Antiaromatic and Open-Shell Character of Dibenzo[<i>a,f</i>]pentalene by Employing Three Strategies: Additional Benzoannulation, BN/CC Isosterism, and Substitution. <i>Chemistry - A European Journal</i> , 2019, 25, 9747-9757. | 1.7 | 19 |
| 12841 | On the spectral profile change in the Q band absorption spectra of metalloporphyrins (Mg, Zn, and) <i>Tj ETQq0 0 0 rgBT /Overlçk 10 Tf 5</i> | 1.2 | 10 |
| 12842 | Mechanisms and Activity of α -Phenylethanol Dehydrogenation Catalyzed by Bifunctional NHC ^{III} Complex. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 3929-3936. | 1.2 | 4 |
| 12843 | Potential antidiabetic zinc(II) complexes of novel 5-oxo-2-thioxopyrrolidine derivatives synthesized via an unprecedented reaction. <i>Tetrahedron Letters</i> , 2019, 60, 1534-1537. | 0.7 | 0 |
| 12844 | The FELion cryogenic ion trap beam line at the FELIX free-electron laser laboratory: infrared signatures of primary alcohol cations. <i>Faraday Discussions</i> , 2019, 217, 172-202. | 1.6 | 40 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12845 | Polyacenes and diffuse interstellar bands. <i>Astronomy and Astrophysics</i> , 2019, 625, A41. | 2.1 | 28 |
| 12846 | In Silico Investigation of the Aggregation-Induced Quenching: the α -Tolane-Based Molecule Case. <i>ChemPhotoChem</i> , 2019, 3, 794-803. | 1.5 | 5 |
| 12847 | Simulation studies of the characteristics of nitrogen-containing additive molecules for solar cells. <i>Chemical Papers</i> , 2019, 73, 2341-2351. | 1.0 | 3 |
| 12848 | C-C coupling at a zeolite-supported Rh(κ -Cp) complex. DFT search for the mechanism. <i>Catalysis Science and Technology</i> , 2019, 9, 2781-2793. | 2.1 | 8 |
| 12849 | Metal-coordination driven intramolecular twisting: a turn-on fluorescent-redox probe for Hg ²⁺ ions through the interaction of ferrocene nonbonding orbitals and dibenzylidenehydrazine. <i>Dalton Transactions</i> , 2019, 48, 8209-8220. | 1.6 | 10 |
| 12850 | A non-conjugated polyethylenimine copolymer-based unorthodox nanoprobe for bioimaging and related mechanism exploration. <i>Biomaterials Science</i> , 2019, 7, 3016-3024. | 2.6 | 20 |
| 12851 | Influence of capping ligands on the assembly of quantum dots and their properties. <i>Materials Science and Technology</i> , 2019, 35, 1053-1060. | 0.8 | 4 |
| 12853 | Quantum-chemical studies of homoleptic iridium(III) complexes in OLEDs: fac versus mer isomers. <i>Journal of Molecular Modeling</i> , 2019, 25, 154. | 0.8 | 7 |
| 12854 | Through-space Spin Coupling in a Silver(II) Porphyrin Dimer upon Stepwise Oxidations: Ag II \rightarrow Ag II ⁺ , Ag II ⁺ \rightarrow Ag III, and Ag III \rightarrow Ag III Metallophilic Interactions. <i>Chemistry - A European Journal</i> , 2019, 25, 10098-10110. | 1.7 | 19 |
| 12855 | A Lieb-like lattice in a covalent-organic framework and its Stoner ferromagnetism. <i>Nature Communications</i> , 2019, 10, 2207. | 5.8 | 67 |
| 12856 | REMP: A hybrid perturbation theory providing improved electronic wavefunctions and properties. <i>Journal of Chemical Physics</i> , 2019, 150, 124107. | 1.2 | 4 |
| 12857 | Molecular docking and spectroscopic studies on the interaction of new fifth-generation antibacterial drug ceftobiprole with calf thymus DNA. <i>Nucleosides, Nucleotides and Nucleic Acids</i> , 2019, 38, 732-751. | 0.4 | 3 |
| 12858 | Gauging the Redox Non-Innocence of a Highly π -Acidic Bis-Tetrazine Pincer Ligand. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 2535-2542. | 1.0 | 2 |
| 12859 | Molecular structure and electronic properties of substituted tetrabenzocoronenes: DFT and TD-DFT investigations. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3970. | 0.9 | 7 |
| 12860 | The fate of rhenium in polyaminocarboxy solution: Hourglass crystal and its speciation study. <i>Journal of Hazardous Materials</i> , 2019, 375, 78-85. | 6.5 | 6 |
| 12861 | Application of the α -inverted chirality columns approach for the monitoring of asymmetric synthesis protocols. <i>Talanta</i> , 2019, 203, 147-152. | 2.9 | 8 |
| 12862 | Exact subsystem time-dependent density-functional theory. <i>Journal of Chemical Physics</i> , 2019, 150, 181101. | 1.2 | 30 |
| 12863 | Aqueous reactions of organic triplet excited states with atmospheric alkenes. <i>Atmospheric Chemistry and Physics</i> , 2019, 19, 5021-5032. | 1.9 | 16 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12864 | Atomic-scale insights into zeolite-based catalysis in N ₂ O decomposition. <i>Science of the Total Environment</i> , 2019, 673, 266-271. | 3.9 | 15 |
| 12865 | Highly Lithiophilic Graphdiyne Nanofilm on 3D Free-Standing Cu Nanowires for High-Energy-Density Electrodes. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 17678-17685. | 4.0 | 32 |
| 12866 | Confining an Ag ₁₀ Core in an Ag ₁₂ Shell: A Four-Electron Superatom with Enhanced Photoluminescence upon Crystallization. <i>ACS Nano</i> , 2019, 13, 5753-5759. | 7.3 | 70 |
| 12867 | A novel structure of grid spirofluorene: a new organic semiconductor with low reorganization energy. <i>New Journal of Chemistry</i> , 2019, 43, 7790-7796. | 1.4 | 14 |
| 12868 | Aryl C=O oxidative addition of phenol derivatives to nickel supported by an N-heterocyclic carbene <i>via</i> a Ni ⁰ five-centered complex. <i>Dalton Transactions</i> , 2019, 48, 7817-7827. | 1.6 | 12 |
| 12869 | Analytical energy gradients for ionized states using equation-of-motion coupled-cluster theory with spin-orbit coupling. <i>Journal of Chemical Physics</i> , 2019, 150, 154114. | 1.2 | 6 |
| 12870 | Efficiently evaluating the Krieger-Li-Iafrate and common-energy-denominator approximations in the frequency-dependent Sternheimer scheme. <i>Physical Review A</i> , 2019, 99, . | 1.0 | 3 |
| 12871 | Long-range screened hybrid-functional theory satisfying the local-density linear response. <i>Physical Review A</i> , 2019, 99, . | 1.0 | 16 |
| 12872 | Cytotoxic polyphenolic compounds from <i>Lespedeza bicolor</i> stem bark. <i>Fitoterapia</i> , 2019, 135, 64-72. | 1.1 | 10 |
| 12873 | Copper-catalyzed N-F Bond Activation for Uniform Intramolecular C-H Amination Yielding Pyrrolidines and Piperidines. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 8912-8916. | 7.2 | 71 |
| 12874 | Sigma bond activation of deuterium mediated by atomic cerium cations: Experiment and theory. <i>International Journal of Mass Spectrometry</i> , 2019, 441, 19-24. | 0.7 | 2 |
| 12875 | Eine Kupfer-katalysierte N-F-Bindungsaktivierung für die einheitliche intramolekulare C-H-Aminierung zu Pyrrolidinen und Piperidinen. <i>Angewandte Chemie</i> , 2019, 131, 9004-9009. | 1.6 | 13 |
| 12876 | Methodological Survey of Simplified TD-DFT Methods for Fast and Accurate Interpretation of UV-Vis-NIR Spectra of Phthalocyanines. <i>ACS Omega</i> , 2019, 4, 7265-7284. | 1.6 | 86 |
| 12877 | A generally applicable atomic-charge dependent London dispersion correction. <i>Journal of Chemical Physics</i> , 2019, 150, 154122. | 1.2 | 697 |
| 12878 | A convenient room temperature <i>ipso</i> -nitration of arylboronic acid catalysed by molecular iodine using zirconium oxynitrate as nitrating species: An experimental and theoretical investigation. <i>Applied Organometallic Chemistry</i> , 2019, 33, e4951. | 1.7 | 1 |
| 12879 | Functional insights of a molecular complex pyrazolium 3,5-dinitrobenzoate:3,5-dinitrobenzoic acid on infectious agents and ctDNA - A comparative biological screening and complementary theoretical calculations. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2019, 196, 111497. | 1.7 | 2 |
| 12880 | Unravelling the Origins of Hydroboration Chemoselectivity Inversion Using an N,O-Chelated Ir(I) Complex: A Computational Study. <i>Journal of Organic Chemistry</i> , 2019, 84, 6709-6718. | 1.7 | 10 |
| 12881 | Reshuffling of Electronic Environment by Introducing CH ₃ NH ₂ ⁺ as an Organic Cation for Enhanced Power Conversion Efficiency and Stability of the Designed Hybrid Organic-Inorganic Perovskite. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13385-13393. | 1.5 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12882 | Insights into Direct Methods for Predictions of Ionization Potential and Electron Affinity in Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2692-2699. | 2.1 | 16 |
| 12883 | Hydrogen quenches the size effects in carbon clusters. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10402-10410. | 1.3 | 3 |
| 12884 | Fiber-Enhanced Raman Gas Spectroscopy for ¹⁸ O- ¹³ C-Labeling Experiments. <i>Analytical Chemistry</i> , 2019, 91, 7562-7569. | 3.2 | 49 |
| 12885 | Molecular Rectifiers on Silicon: High Performance by Enhancing Top-Electrode/Molecule Coupling. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 18564-18570. | 4.0 | 21 |
| 12886 | Mechanistic insights into silver(I)-mediated trifluoromethylation of aryldiazonium salts. <i>Computational and Theoretical Chemistry</i> , 2019, 1158, 15-21. | 1.1 | 1 |
| 12887 | Adsorption and dissociation of iron phthalocyanine on H/Si(111): Impact of van der Waals interactions and perspectives for subsurface doping. <i>Physical Review B</i> , 2019, 99, . | 1.1 | 6 |
| 12888 | The Influence of the Electronic Structure Method on Intersystem Crossing Dynamics. The Case of Thioformaldehyde. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3470-3480. | 2.3 | 30 |
| 12889 | [Ni ₃ (Pr ₂ Im) ₃ (μ ² -CO) ₃ (μ ³ -CO)] ⁺ A CO-Stabilized NHC Analogue of the Parent Neutral Nickel Chini-Type Cluster. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 2618-2623. | 1.0 | 17 |
| 12890 | Direct Access to IMes ^F and IMes ^F ₂ by Electrophilic Fluorination of Abnormal N-Heterocyclic Carbenes. <i>Organometallics</i> , 2019, 38, 2330-2337. | 1.1 | 19 |
| 12891 | C-N Bond Rotation Controls Photoinduced Electron Transfer in an Aminostyrene-Stilbene Donor-Acceptor System. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4333-4341. | 1.1 | 4 |
| 12892 | Account of chemical bonding and enhanced reactivity of vanadium-doped rhodium clusters toward C-H activation: a DFT investigation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9935-9948. | 1.3 | 8 |
| 12893 | Transition metal catalysed C7 and ortho-selective halogenation of 2-arylbenzo[d]oxazoles. <i>Organic Chemistry Frontiers</i> , 2019, 6, 2226-2233. | 2.3 | 18 |
| 12894 | Scrutinizing metal-ligand covalency and redox non-innocence via nitrogen K-edge X-ray absorption spectroscopy. <i>Chemical Science</i> , 2019, 10, 5044-5055. | 3.7 | 29 |
| 12895 | Synthesis, Crystal Structure, Thermal Analysis, and DFT Calculations of Molecular Copper(II) Chloride Complexes with Bitopic Ligand 1,1,2,2-tetrakis(pyrazol-1-yl)ethane. <i>Crystals</i> , 2019, 9, 222. | 1.0 | 1 |
| 12896 | Molecular Dynamics Simulations on Relaxed Reduced-Dimensional Potential Energy Surfaces. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4543-4554. | 1.1 | 5 |
| 12897 | A Theoretical Study on Divalent Heavier Group 14 Complexes as Promising Donor Ligands for Building Uranium-Metal Bonds. <i>Organometallics</i> , 2019, 38, 1963-1972. | 1.1 | 10 |
| 12898 | Understanding the Solution Chemistry of Lead Halide Perovskites Precursors. <i>ACS Applied Energy Materials</i> , 2019, 2, 3400-3409. | 2.5 | 74 |
| 12899 | Philicity of Acetonyl and Benzoyl Radicals: A Comparative Experimental and Computational Study. <i>Chemistry - A European Journal</i> , 2019, 25, 9088-9097. | 1.7 | 16 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12900 | Polar Bilayer Cathode for Advanced Lithium–Sulfur Battery: Synergy Between Polysulfide Conversion and Confinement. <i>Journal of Physical Chemistry C</i> , 2019, 123, 10777-10787. | 1.5 | 13 |
| 12901 | Intramolecular [2+2] Photocycloaddition of Cyclic Enones: Selectivity Control by Lewis Acids and Mechanistic Implications. <i>Chemistry - A European Journal</i> , 2019, 25, 8135-8148. | 1.7 | 45 |
| 12902 | Determination of the best functional and basis sets for optimization of the structure of hypervalent iodines and calculation of their first and second bond dissociation enthalpies. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3961. | 0.9 | 26 |
| 12903 | A photoelectron imaging and quantum chemistry study of the deprotonated cyan fluorescent protein chromophore anion. <i>Molecular Physics</i> , 2019, 117, 3027-3035. | 0.8 | 3 |
| 12904 | Performance of 3D-RISM-KH in Predicting Hydration Free Energy: Effect of Solute Parameters. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4087-4093. | 1.1 | 26 |
| 12905 | Vanadyl Porphyrin Speciation Based on Submegahertz Ligand Proton Hyperfine Couplings. <i>Energy & Fuels</i> , 2019, 33, 4237-4243. | 2.5 | 19 |
| 12906 | Imaging covalent bond formation by H atom scattering from graphene. <i>Science</i> , 2019, 364, 379-382. | 6.0 | 76 |
| 12907 | An anomalous addition of chlorosulfonyl isocyanate to a carbonyl group: the synthesis of ((3a <i>S</i> ,7a <i>R</i> , <i>E</i>)-2-ethyl-3-oxo-2,3,3a,4,7,7a-hexahydro-1 <i>H</i> -isoindol-1-ylidene)sulfamoyl chloride. <i>Beilstein Journal of Organic Chemistry</i> , 2019, 15, 931-936. | 1.3 | 2 |
| 12908 | Thermal properties of protic ionic liquids derivatives triethanolamine-based salts of mineral and organic acids. <i>Journal of Thermal Analysis and Calorimetry</i> , 2019, 138, 703-712. | 2.0 | 4 |
| 12909 | Enrichment mechanisms of antimony and arsenic in marine ferromanganese oxides: Insights from the structural similarity. <i>Geochimica Et Cosmochimica Acta</i> , 2019, 257, 110-130. | 1.6 | 25 |
| 12910 | Complexes of Co(II), Ni(II), and Cu(II) with (Z)-10-(2-(4-Amino-5-Thioxo-4,5-Dihydro-1 <i>H</i> -1,2,4-Triazol-3-yl)hydrazono)-9-Phenanthrone: Synthesis, Spectral Studies, and Quantum Chemical Simulation of the Structures. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2019, 45, 1-10. | 0.3 | 0 |
| 12911 | Mass spectrometry evidence for self-rigidification of π -conjugated oligomers containing 3,4-ethylenedioxythiophene groups using RRKM theory and internal energy calibration. <i>European Journal of Mass Spectrometry</i> , 2019, 25, 239-250. | 0.5 | 0 |
| 12912 | Crystal Structure, Sensitiveness and Theoretical Explosive Performance of Xylitol Pentanitrate (XPN). <i>Propellants, Explosives, Pyrotechnics</i> , 2019, 44, 541-549. | 1.0 | 10 |
| 12913 | Unraveling the molecular mechanisms of color expression in anthocyanins. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8757-8766. | 1.3 | 20 |
| 12914 | Plasmon damping depends on the chemical nature of the nanoparticle interface. <i>Science Advances</i> , 2019, 5, eaav0704. | 4.7 | 128 |
| 12916 | Concise Synthesis of a New Chiral Cyclopentenone Building Block for Prostaglandins and their Derivatives. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 2612-2620. | 1.2 | 1 |
| 12917 | Theoretical insights into the sensing mechanism of a series of terpyridine-based chemosensors for TNP. <i>Chemical Physics Letters</i> , 2019, 725, 45-51. | 1.2 | 15 |
| 12918 | Micromechanism study on electronic and magnetic properties of silicene regulated by oxygen. <i>Journal of Materials Science and Technology</i> , 2019, 35, 1803-1808. | 5.6 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12919 | High-Frequency and -Field EPR (HFEPFR) Investigation of a Pseudotetrahedral Cr ^{IV} Siloxide Complex and Computational Studies of Related Cr ^{IV} L ₄ Systems. <i>Inorganic Chemistry</i> , 2019, 58, 4907-4920. | 1.9 | 11 |
| 12920 | On the formation of phosphorous polycyclic aromatics hydrocarbons (PAHs) in astrophysical environments. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8015-8021. | 1.3 | 8 |
| 12921 | Learning from Failure: Predicting Electronic Structure Calculation Outcomes with Machine Learning Models. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2331-2345. | 2.3 | 66 |
| 12922 | The Metal Hydride Problem of Computational Chemistry: Origins and Consequences. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2888-2900. | 1.1 | 26 |
| 12923 | Computational studies, NMR, Raman and infrared spectral analysis of centrosymmetric (2Z,4Z)-Hexa-2,4-dienedinitrile. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1950011. | 1.8 | 3 |
| 12924 | Mechanistic Details on the Conversion of Si ^{IV} -O to Si ^{IV} -C Bonds Using Metal Hydrides: A Density Functional Theory Study. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 1335-1342. | 1.0 | 1 |
| 12925 | Segregation of tetracarbon units in low-energy tetracarbendane structures: Major differences from their aluminum and gallium analogs. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25934. | 1.0 | 0 |
| 12926 | The Electronic Determinants of Spin Crossover Described by Density Functional Theory. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 1-33. | 0.6 | 2 |
| 12927 | Depth Distribution of Spin-Labeled Liponitroxides within Lipid Bilayers: A Combined EPR and Molecular Dynamics Approach. <i>ACS Omega</i> , 2019, 4, 5029-5037. | 1.6 | 16 |
| 12928 | Characterization of a trans-trans Carbonic Acid-Fluoride Complex by Infrared Action Spectroscopy in Helium Nanodroplets. <i>Journal of the American Chemical Society</i> , 2019, 141, 5815-5823. | 6.6 | 18 |
| 12929 | Cross Conjugation in Polyenes and Related Hydrocarbons: What Can Be Learned from Valence Bond Theory about Single-Molecule Conductance?. <i>Journal of the American Chemical Society</i> , 2019, 141, 6030-6047. | 6.6 | 26 |
| 12930 | The Effect of Cofactor Binding on the Conformational Plasticity of the Biological Receptors in Artificial Metalloenzymes: The Case Study of LmrR. <i>Frontiers in Chemistry</i> , 2019, 7, 211. | 1.8 | 9 |
| 12931 | Rapid synthesis of 4-alkynyl coumarins and tunable electronic properties of emission solvatochromic fluorophores. <i>Dyes and Pigments</i> , 2019, 166, 357-366. | 2.0 | 19 |
| 12932 | Polyaniline/chitosan as a corrosion inhibitor for mild steel in acidic medium. <i>RSC Advances</i> , 2019, 9, 9211-9217. | 1.7 | 69 |
| 12933 | Mechanistic insights into the catalytic transfer hydrogenation of furfural with methanol and alkaline earth oxides. <i>Journal of Catalysis</i> , 2019, 372, 61-73. | 3.1 | 44 |
| 12934 | Structure and vibrational spectra of p-coumaric acid dimers by DFT methods. <i>Vibrational Spectroscopy</i> , 2019, 101, 100-108. | 1.2 | 6 |
| 12935 | How Does the Redox State of Polyoxovanadates Influence the Collective Behavior in Solution? A Case Study with [V ₁₈ O ₄₂]q ⁿ⁻ (q = 3, 5, 7, 11, and 13). <i>Inorganic Chemistry</i> , 2019, 58, 3881-3894. | 1.9 | 18 |
| 12936 | Designing in the Face of Uncertainty: Exploiting Electronic Structure and Machine Learning Models for Discovery in Inorganic Chemistry. <i>Inorganic Chemistry</i> , 2019, 58, 10592-10606. | 1.9 | 79 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12937 | Searching for stable fullerenes in space with computational chemistry. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019, 485, 1137-1146. | 1.6 | 23 |
| 12938 | 1,3- Δ Diphosphacyclobutene Cobalt Complexes. <i>Chemistry - A European Journal</i> , 2019, 25, 6180-6188. | 1.7 | 7 |
| 12939 | Ultrafast Intramolecular and Solvation Dynamics in 4,7-Bis(4,5-dibutylbenzo[1,2- <i>b</i> :4,3- <i>b'</i>]-bisthiophene[1,2- <i>b</i> :4,3- <i>b'</i>]-bisthiophen-2-yl)-2,1,3-benzothiadiazole. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5840-5852. | 1.5 | 11 |
| 12940 | Effect of Electronic Coupling on Electron Transfer Rates from Photoexcited Naphthalenediimide Radical Anion to $\text{Re}(\text{bpy})(\text{CO})_3\text{X}$. <i>Journal of Physical Chemistry C</i> , 2019, 123, 10178-10190. | 1.5 | 10 |
| 12941 | Transport and Optical Gaps in Amorphous Organic Molecular Materials. <i>Molecules</i> , 2019, 24, 609. | 1.7 | 0 |
| 12942 | Low-Barrier Hydrogen Bonds in Negative Thermal Expansion Material $\text{H}_3[\text{Co}(\text{CN})_6]$. <i>Chemistry - A European Journal</i> , 2019, 25, 6814-6822. | 1.7 | 14 |
| 12943 | Evaluation of the antioxidant potential of myricetin 3-O- β -L-rhamnopyranoside and myricetin 4-O- β -L-rhamnopyranoside through a computational study. <i>Journal of Molecular Modeling</i> , 2019, 25, 89. | 0.8 | 37 |
| 12944 | Hirshfeld surface analysis, vibrational spectra, optical, DFT studies and biological activities of $(\text{C}_7\text{H}_{12}\text{N}_2)_2[\text{SnCl}_6]\text{Cl}_2 \cdot 1.5\text{H}_2\text{O}$ compound. <i>Chemical Physics Letters</i> , 2019, 722, 160-172. | 1.2 | 13 |
| 12945 | Monitoring an ionic liquid synthesis with in-situ IR-spectroscopy – The intricacy of solvent effects. <i>Chemical Engineering Journal</i> , 2019, 368, 649-658. | 6.6 | 3 |
| 12946 | Platinum(II) and copper(II) complexes of 7-azaindole-3-carboxaldehyde: crystal structures, IR and Raman spectra, DFT calculations and in vitro antiproliferative activity of the platinum(II) complex. <i>Inorganica Chimica Acta</i> , 2019, 490, 68-77. | 1.2 | 10 |
| 12947 | Anharmonicity of Vibrational Modes in Hydrogen Chloride–Water Mixtures. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2535-2547. | 2.3 | 5 |
| 12948 | Quantum chemical calculations of the thermochemistry of tantalum oxyhydroxide species. <i>Journal of the American Ceramic Society</i> , 2019, 102, 3836-3842. | 1.9 | 6 |
| 12949 | Pyridinium p-DSSC dyes: An old acceptor learns new tricks. <i>Dyes and Pigments</i> , 2019, 165, 508-517. | 2.0 | 18 |
| 12950 | A DFT study on the mechanism of rhodium-catalyzed regioselective hydrothiolation of the allyl amine. <i>Molecular Catalysis</i> , 2019, 468, 62-74. | 1.0 | 3 |
| 12951 | Examination of the electronic structure of oxygen-containing PAH dimers and trimers. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 903-910. | 2.4 | 11 |
| 12952 | Planar rings in nano-Saturns and related complexes. <i>Chemical Communications</i> , 2019, 55, 3650-3653. | 2.2 | 13 |
| 12953 | Biological Activity and In Silico Study of 3-Modified Derivatives of Betulin and Betulinic Aldehyde. <i>International Journal of Molecular Sciences</i> , 2019, 20, 1372. | 1.8 | 12 |
| 12954 | Evaluation of DFT Methods and Implicit Solvation Models for Anion–Binding Host–Guest Systems. <i>Helvetica Chimica Acta</i> , 2019, 102, e1900032. | 1.0 | 13 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12955 | Structural Evolution and Chemical Bonding in Bi-nuclear Niobium Sulfide Clusters: Nb ₂ S _n (n=4-7). Journal of Cluster Science, 2019, 30, 735-746. | 1.7 | 1 |
| 12956 | New phosphate derivatives of betulin as anticancer agents: Synthesis, crystal structure, and molecular docking study. Bioorganic Chemistry, 2019, 87, 613-628. | 2.0 | 24 |
| 12957 | Discovery of Small Molecules that Activate RNA Methylation through Cooperative Binding to the METTL3-14-WTAP Complex Active Site. Cell Reports, 2019, 26, 3762-3771.e5. | 2.9 | 121 |
| 12958 | The importance of diffuse functions in basis sets to produce reliable 3D pictures of dual descriptor. Chemical Physics Letters, 2019, 724, 29-34. | 1.2 | 5 |
| 12959 | Rotational spectra of the low energy conformers observed in the (1R)-myrtenol monomer. Journal of Molecular Spectroscopy, 2019, 356, 32-36. | 0.4 | 14 |
| 12960 | Density Functional Theory Study of the Capture and Release of Carbon Dioxide by Benzyl Disulfide, α -Diselenide, and α -Ditelluride. Journal of Physical Chemistry A, 2019, 123, 3383-3388. | 1.1 | 4 |
| 12961 | Self-Organization of PEDOT:PSS Induced by Green and Water-Soluble Organic Molecules. Journal of Physical Chemistry C, 2019, 123, 9745-9755. | 1.5 | 32 |
| 12962 | Comparative Computational Study of Electronic Excitations of Neutral and Charged Small Oligothiophenes and Their Extrapolations Based on Simple Models. ACS Omega, 2019, 4, 5758-5767. | 1.6 | 4 |
| 12963 | Twist-bend nematic liquid crystals based on thioether linkage. New Journal of Chemistry, 2019, 43, 6786-6793. | 1.4 | 52 |
| 12964 | Photoactivated cell-killing involving a low molecular weight, donor-acceptor diphenylacetylene. Chemical Science, 2019, 10, 4673-4683. | 3.7 | 17 |
| 12965 | Triphenylamine-substituted 2-pyridyl-1,2,3-triazole copper(I) complexes: an experimental and computational investigation. Journal of Coordination Chemistry, 2019, 72, 1378-1394. | 0.8 | 8 |
| 12966 | Universal nature of different methods of obtaining the exact Kohn-Sham exchange-correlation potential for a given density. Journal of Physics B: Atomic, Molecular and Optical Physics, 2019, 52, 075007. | 0.6 | 16 |
| 12967 | Systematic study of relativistic and chemical enhancements of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi mathvariant="script"} \rangle P \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle, \langle \text{mml:mi} \rangle \langle \text{mml:mi mathvariant="script"} \rangle T \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$ -odd effects in polar diatomic radicals. Physical Review A, 2019, 99, . | 1.0 | 24 |
| 12968 | Raman spectra of rare earth double-decker complexes with porphyrinato and 2,3-naphthalocyaninato ligands. Journal of Porphyrins and Phthalocyanines, 2019, 23, 260-266. | 0.4 | 0 |
| 12969 | Palladium complexes with 3-methyl-8-thia-1,3-diaza-spiro[4.5]decane-2,4-dione: experimental and theoretical studies. Arkivoc, 2019, 2018, 398-406. | 0.3 | 2 |
| 12970 | A computational study on the reaction between fisetin and 2,2-diphenyl-1-picrylhydrazyl (DPPH). Journal of Molecular Modeling, 2019, 25, 103. | 0.8 | 28 |
| 12971 | Novel aluminum complexes bearing 2-(aminomethylene)malonate ligands with high efficiency and controllability in ring-opening polymerization of β -caprolactone. European Polymer Journal, 2019, 115, 399-408. | 2.6 | 11 |
| 12972 | Synthesis and structural DFT studies of Ni(II) and Co(II) complexes with s-triazine-based di-compartmental ligand. Polyhedron, 2019, 165, 162-170. | 1.0 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 12973 | A Known Iron(II) Complex in Different Nanosized Particles: Variable-Temperature Raman Study of Its Spin-Crossover Behavior. <i>Inorganic Chemistry</i> , 2019, 58, 5183-5195. | 1.9 | 9 |
| 12974 | Câ€F activation of perfluorophenazine at nickel: selectivity and mechanistic investigations. <i>Dalton Transactions</i> , 2019, 48, 6153-6161. | 1.6 | 4 |
| 12975 | Redox activity of nickel and vanadium porphyrins: a possible mechanism behind petroleum genesis and maturation?. <i>RSC Advances</i> , 2019, 9, 9509-9516. | 1.7 | 15 |
| 12976 | Structure elucidation of cyclohexene (9Z)-octadec-9-enyl ethers isolated from the leaves of <i>Uvaria cherreensis</i> (Annonaceae). <i>Tetrahedron</i> , 2019, 75, 2336-2342. | 1.0 | 5 |
| 12977 | ¹³ C NMR Shifts as an Indicator of Uâ€C Bond Covalency in Uranium(VI) Acetylide Complexes: An Experimental and Computational Study. <i>Inorganic Chemistry</i> , 2019, 58, 4152-4163. | 1.9 | 34 |
| 12978 | Protonation of the Biliverdin IX β Chromophore in the Red and Far-Red Photoactive States of a Bacteriophytochrome. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2325-2334. | 1.2 | 25 |
| 12979 | A concerted addition mechanism in [Hmim]Br-triggered thiolâ€ene reactions: a typical â€œionic liquid effectâ€ revealed by DFT and experimental studies. <i>New Journal of Chemistry</i> , 2019, 43, 5752-5758. | 1.4 | 8 |
| 12980 | Performance of DFT methods in the calculation of isotropic and dipolar contributions to ¹⁴ N hyperfine coupling constants of nitroxide radicals. <i>Journal of Molecular Modeling</i> , 2019, 25, 93. | 0.8 | 9 |
| 12981 | Real-time sensing of lead with epitaxial graphene-integrated microfluidic devices. <i>Sensors and Actuators B: Chemical</i> , 2019, 288, 425-431. | 4.0 | 34 |
| 12982 | Synthesis, characterization, DFT calculations and catalase-like enzymatic activities of novel hexadentate Schiff base and its manganese complexes. <i>Journal of Molecular Structure</i> , 2019, 1186, 250-262. | 1.8 | 12 |
| 12983 | Electron Delocalization in Planar Metallacycles: H $\frac{1}{4}$ ckel or M $\frac{1}{4}$ bius Aromatic?. <i>ChemistryOpen</i> , 2019, 8, 219-227. | 0.9 | 49 |
| 12984 | A theoretical study of the photoelectron spectra of dichloroketene with accurate computation of ionization energies via complete basis set limit extrapolation. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25866. | 1.0 | 6 |
| 12985 | Infrared Spectroscopy and Mass Spectrometry of CO ₂ Clusters during Nucleation and Growth. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2426-2437. | 1.1 | 14 |
| 12986 | Study of the effect of the ligand structure on the catalytic activity of Pd@ ligand decorated halloysite: Combination of experimental and computational studies. <i>Applied Organometallic Chemistry</i> , 2019, 33, e4891. | 1.7 | 57 |
| 12987 | Excited-State Vibrational Frequencies: Restricted Virtual Space Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2949-2956. | 1.1 | 3 |
| 12988 | Novel <i>in situ</i> synthesis of copper nanoparticles supported on reduced graphene oxide and its application as a new catalyst for the decomposition of composite solid propellants. <i>RSC Advances</i> , 2019, 9, 8480-8489. | 1.7 | 29 |
| 12989 | Theoretical Study on the Transition-Metal-Catalyzed Cycloadditions of 2 <i>H</i> -Azirines with Alkynes: Implication of Carbenoid Intermediates. <i>Bulletin of the Chemical Society of Japan</i> , 2019, 92, 619-628. | 2.0 | 3 |
| 12990 | Understanding UVâ€Vis Spectra of Halogenated Tetraazaperopyrenes (TAPPs): A Computational Study. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3160-3169. | 1.1 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 12991 | Cobalt-Catalyzed Asymmetric Synthesis of gem-Bis(silyl)alkanes by Double Hydrosilylation of Aliphatic Terminal Alkynes. <i>CheM</i> , 2019, 5, 881-895. | 5.8 | 99 |
| 12992 | Nanohybrid sensor for simple, cheap, and sensitive electrochemical recognition and detection of methylglyoxal as chemical markers. <i>Journal of Electroanalytical Chemistry</i> , 2019, 839, 177-186. | 1.9 | 11 |
| 12993 | Molecular design of ionic liquids as novel non-metal catalysts for the acetylene hydrochlorination reaction. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7635-7644. | 1.3 | 7 |
| 12994 | Key Mechanistic Features in Palladium-Catalyzed Methylcyclopropanation of Norbornenes With Vinyl Bromides: Insights From DFT Calculations. <i>Frontiers in Chemistry</i> , 2019, 7, 169. | 1.8 | 6 |
| 12995 | Spectroscopic properties of push-pull 2-(4-carboxyphenyl)-6-dimethylaminobenzothiazole derivatives in solution and the solid state. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 376, 324-332. | 2.0 | 3 |
| 12996 | Main-Group-Element Isophlorin Complexes Revisited: The Question of a Subvalent Central Atom. <i>Inorganic Chemistry</i> , 2019, 58, 4634-4640. | 1.9 | 7 |
| 12997 | Evaluating Unexpectedly Short Non-covalent Distances in X-ray Crystal Structures of Proteins with Electronic Structure Analysis. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2199-2211. | 2.5 | 38 |
| 12998 | Polymorphism of hydrogen-bonded star mesogens – a combinatorial DFT-D and FT-IR spectroscopy study. <i>RSC Advances</i> , 2019, 9, 8444-8453. | 1.7 | 5 |
| 12999 | Role of Alkaline-Earth Metal-Catalyst: A Theoretical Study of Pyridines Hydroboration. <i>Frontiers in Chemistry</i> , 2019, 7, 149. | 1.8 | 5 |
| 13000 | Development of Prediction Models on Base-Catalyzed Hydrolysis Kinetics of Phthalate Esters with Density Functional Theory Calculation. <i>Environmental Science & Technology</i> , 2019, 53, 5828-5837. | 4.6 | 41 |
| 13001 | Enhanced Fe-Centered Redox Flexibility in Fe–Ti Heterobimetallic Complexes. <i>Inorganic Chemistry</i> , 2019, 58, 6199-6214. | 1.9 | 29 |
| 13002 | Fast Quantum Chemical Simulations of Infrared Spectra of Organic Compounds with the B97-3c Composite Method. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3802-3808. | 1.1 | 26 |
| 13003 | Performance of the Diffusion Quantum Monte Carlo Method with a Single-Slater-Jastrow Trial Wavefunction Using Natural Orbitals and Density Functional Theory Orbitals on Atomization Energies of the Gaussian-2 Set. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3809-3817. | 1.1 | 12 |
| 13004 | Transient and Enduring Electronic Resonances Drive Coherent Long Distance Charge Transport in Molecular Wires. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1845-1851. | 2.1 | 17 |
| 13005 | Dynamic Reorganization and Confinement of Ti ^{IV} Active Sites Controls Olefin Epoxidation Catalysis on Two-Dimensional Zeotypes. <i>Journal of the American Chemical Society</i> , 2019, 141, 7090-7106. | 6.6 | 68 |
| 13006 | Synthesis and Characterization of Cyclometalated NHC Platinum Complexes with Chelating Carboxylate Ligands. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 2284-2290. | 1.0 | 9 |
| 13007 | TCA self-assembled fluorescence probe for Cu (II) ion based on the unique configuration of extra nuclear electrons of metal ions: A TDDFT study. <i>Computational and Theoretical Chemistry</i> , 2019, 1157, 1-10. | 1.1 | 0 |
| 13008 | Integrated Computational Study of the Cu-Catalyzed Hydration of Alkenes in Water Solvent and into the Context of an Artificial Metallohydratase. <i>ACS Catalysis</i> , 2019, 9, 4616-4626. | 5.5 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13009 | Chain rigidity modification to promote the electrochemical performance of polymeric battery electrode materials. <i>Journal of Materials Chemistry A</i> , 2019, 7, 10581-10588. | 5.2 | 33 |
| 13010 | Thermodynamic and kinetic aspects of glycine and its radical cation under interstellar medium conditions. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019, 486, 2153-2164. | 1.6 | 9 |
| 13011 | Gas-Phase Deconstruction of UO_2^{2+} : Mass Spectrometry Evidence for Generation of $[\text{OU}^+\text{Vl}^+\text{CH}]^+$ by Collision-Induced Dissociation of $[\text{U}^+\text{Vl}^+\text{O}_2^+(\text{C}^+\text{H})]^+$. <i>Journal of the American Society for Mass Spectrometry</i> , 2019, 30, 796-805. | 1.2 | 11 |
| 13012 | Reaction mechanism of non-enzymatic stereoselective formation of wine lactone. <i>Chemical Physics Letters</i> , 2019, 725, 114-118. | 1.2 | 0 |
| 13013 | Hydrazideâ€Hydrazone Small Molecules as AIEgens: Illuminating Mitochondria in Cancer Cells. <i>Chemistry - A European Journal</i> , 2019, 25, 8229-8235. | 1.7 | 26 |
| 13014 | Taming the Complexity of Donorâ€Acceptor Stenhouse Adducts: Infrared Motion Pictures of the Complete Switching Pathway. <i>Journal of the American Chemical Society</i> , 2019, 141, 7376-7384. | 6.6 | 66 |
| 13015 | Long Carbon-Based Chains of Interstellar Medium Can Have a Triplet Ground State. Why Is This Important for Astrochemistry?. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 863-872. | 1.2 | 18 |
| 13016 | Drastic photoluminescence modulation of an organic molecular crystal with high pressure. <i>Materials Chemistry Frontiers</i> , 2019, 3, 1510-1517. | 3.2 | 17 |
| 13017 | A photoswitchable GABA receptor channel blocker. <i>British Journal of Pharmacology</i> , 2019, 176, 2661-2677. | 2.7 | 20 |
| 13018 | Physicochemical properties of the three-cavity form of calix[nâ€%4, 6, 8]aren molecules: DFT investigation. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1. | 0.5 | 3 |
| 13019 | Mapping binary copolymer property space with neural networks. <i>Chemical Science</i> , 2019, 10, 4973-4984. | 3.7 | 36 |
| 13020 | Structural interpretation of the ^{31}P NMR chemical shifts in thiophosphate and phosphate: key effects due to spinâ€orbit and explicit solvent. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9924-9934. | 1.3 | 11 |
| 13021 | Fully numerical Hartreeâ€Fock and density functional calculations. II. Diatomic molecules. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25944. | 1.0 | 22 |
| 13022 | Evaluating Transition Metal Barrier Heights with the Latest Density Functional Theory Exchangeâ€Correlation Functionals: The MOBH35 Benchmark Database. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3761-3781. | 1.1 | 104 |
| 13023 | Laboratory EXAFS determined structure of the stable complexes in the ternary $\text{Ni}(\text{EDTA})^-\text{CN}^+$ system. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9239-9245. | 1.3 | 4 |
| 13024 | Methyl Thioether Functionalization of a Polymeric Donor for Efficient Solar Cells Processed from Non-Halogenated Solvents. <i>Chemistry of Materials</i> , 2019, 31, 3025-3033. | 3.2 | 23 |
| 13025 | Transition state analysis of an enantioselective Michael addition by a bifunctional thiourea organocatalyst. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 3934-3939. | 1.5 | 19 |
| 13026 | High-level theoretical benchmark investigations of the UV-vis absorption spectra of paradigmatic polycyclic aromatic hydrocarbons as models for graphene quantum dots. <i>Journal of Chemical Physics</i> , 2019, 150, 124302. | 1.2 | 35 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 13027 | Light-activated ruthenium (II)-bicalutamide prodrugs for prostate cancer. <i>Journal of Inorganic Biochemistry</i> , 2019, 196, 110684. | 1.5 | 19 |
| 13028 | Spectroscopic and electrophoresis study of substitution on the surface of gold nanoparticles by different mercaptoalkyl carboxylic acids and bioconjugation with bovine serum albumin. <i>Analytical and Bioanalytical Chemistry</i> , 2019, 411, 3047-3058. | 1.9 | 5 |
| 13029 | Relativistic corrections to the electric field gradient given by linear response elimination of the small component formalism. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25935. | 1.0 | 4 |
| 13030 | Different mutual positions of double bonds in open carbon chains and corresponding information from magnetically induced current densities. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25941. | 1.0 | 2 |
| 13031 | A quantum chemical study of the effect of substituents in governing the strength of the Sâ€“F bonds of sulfenyl-type fluorides toward homolytic dissociation and fluorine atom transfer. <i>Chemical Data Collections</i> , 2019, 20, 100186. | 1.1 | 5 |
| 13032 | Effect of organic cation states on electronic properties of mixed organicâ€“inorganic halide perovskite clusters. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8161-8169. | 1.3 | 10 |
| 13033 | The Puzzling Monopentamethylcyclopentadienyltitanium(III) Dichloride Reagent: Structure and Properties. <i>Inorganic Chemistry</i> , 2019, 58, 5314-5324. | 1.9 | 9 |
| 13034 | Di-tert-butylcatecholate derivatives of titanocene. <i>New Journal of Chemistry</i> , 2019, 43, 6636-6642. | 1.4 | 1 |
| 13035 | Stereoisomer specific reaction of hexabromocyclododecane with reduced sulfur species in aqueous solutions. <i>Chemosphere</i> , 2019, 226, 238-245. | 4.2 | 12 |
| 13036 | ¹ H high field electron-nuclear double resonance spectroscopy at 263â€“GHz/9.4â€“T. <i>Journal of Magnetic Resonance</i> , 2019, 303, 17-27. | 1.2 | 19 |
| 13037 | Tetraalkylammonium Salts of Platinum Nitrate Complexes: Isolation, Structure, and Relevance to the Preparation of PtO ₂ /CeO ₂ Catalysts for Low-Temperature CO Oxidation. <i>Inorganic Chemistry</i> , 2019, 58, 6075-6087. | 1.9 | 27 |
| 13038 | State-Dependent Fragmentation of Protonated Uracil and Uridine. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3551-3557. | 1.1 | 7 |
| 13039 | A universal density matrix functional from molecular orbital-based machine learning: Transferability across organic molecules. <i>Journal of Chemical Physics</i> , 2019, 150, 131103. | 1.2 | 88 |
| 13040 | Data Science Based Mg Corrosion Engineering. <i>Frontiers in Materials</i> , 2019, 6, . | 1.2 | 34 |
| 13041 | Efficient implementation of the analytical second derivatives of hartreeâ€“fock and hybrid DFT energies within the framework of the conductorâ€“like polarizable continuum model. <i>Journal of Computational Chemistry</i> , 2019, 40, 1816-1828. | 1.5 | 31 |
| 13042 | Structure and adhesion energy of the (10.4) calcite/(001) ice Ih and (210) baryte/(001) ice Ih interfaces. <i>CrystEngComm</i> , 2019, 21, 2920-2928. | 1.3 | 3 |
| 13043 | Electrochemical sensing of ecstasy with electropolymerized molecularly imprinted poly(o-phenylenediamine) polymer on the surface of disposable screen-printed carbon electrodes. <i>Sensors and Actuators B: Chemical</i> , 2019, 290, 378-386. | 4.0 | 77 |
| 13044 | Twist and Degradeâ€“Impact of Molecular Structure on the Photostability of Nonfullerene Acceptors and Their Photovoltaic Blends. <i>Advanced Energy Materials</i> , 2019, 9, 1803755. | 10.2 | 95 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13045 | Franckâ€“Condon Blockade and Aggregationâ€“Modulated Conductance in Molecular Devices Using Aggregationâ€“Induced Emissionâ€“Active Molecules. <i>Angewandte Chemie</i> , 2019, 131, 6012-6016. | 1.6 | 6 |
| 13046 | Magnetic, electronic, ferroelectric, structural and topological analysis of AlFeO ₃ , FeAlO ₃ , FeVO ₃ , BiFeO ₃ and PbFeO ₃ materials: Theoretical evidences of magnetoelectric coupling. <i>Journal of Magnetism and Magnetic Materials</i> , 2019, 480, 199-208. | 1.0 | 27 |
| 13047 | Advances in Density-Functional Calculations for Materials Modeling. <i>Annual Review of Materials Research</i> , 2019, 49, 1-30. | 4.3 | 87 |
| 13048 | Determination of Reaction Rate Coefficients in Free-Radical Polymerization Using Density Functional Theory. , 2019, , 47-98. | | 6 |
| 13049 | Ion-pair complexes of Schiff base Fe(III) cations and complex anions. <i>New Journal of Chemistry</i> , 2019, 43, 4937-4946. | 1.4 | 4 |
| 13050 | 4-aminoazobenzene modified natural glucomannan as a green eco-friendly inhibitor for the mild steel in 0.5 M HCl solution. <i>Corrosion Science</i> , 2019, 151, 132-142. | 3.0 | 128 |
| 13051 | Phosphonic acid and alkyl phosphate-derivatized resins for the simultaneous concentration and detection of uranium in environmental waters. <i>Reactive and Functional Polymers</i> , 2019, 137, 133-139. | 2.0 | 20 |
| 13052 | Spectroscopic and quantum chemical study of difluoroboron β^2 -diketonate luminophores: Isomeric acetylaphtholate chelates. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 214, 67-78. | 2.0 | 6 |
| 13053 | Ionization and fragmentation of uracil upon microhydration. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4810-4821. | 1.3 | 10 |
| 13054 | Many-Body Quantum Monte Carlo Study of 2D Materials: Cohesion and Band Gap in Single-Layer Phosphorene. <i>Physical Review X</i> , 2019, 9, . | 2.8 | 27 |
| 13055 | Relativistic Effects on a Metalâ€“Metal Bond: Osmium Corrole Dimers. <i>Inorganic Chemistry</i> , 2019, 58, 2798-2806. | 1.9 | 14 |
| 13056 | Theoretical Rationalization of the Dual Photophysical Behavior of C ₆₀ ⁺ . <i>Journal of Physical Chemistry A</i> , 2019, 123, 1824-1829. | 1.1 | 7 |
| 13057 | Benchmarking Density Functional Theory Functionals for Polarons in Oxides: Properties of CeO ₂ . <i>Journal of Physical Chemistry C</i> , 2019, 123, 5164-5175. | 1.5 | 28 |
| 13058 | <i>i</i> -Wittig Reaction with Nitriles: How Carbonyl Function Switches from Reacting to Activating. <i>Organic Letters</i> , 2019, 21, 1087-1092. | 2.4 | 25 |
| 13059 | Predicting the Outcome of Photocyclisation Reactions: A Joint Experimental and Computational Investigation. <i>Chemistry - an Asian Journal</i> , 2019, 14, 1293-1303. | 1.7 | 3 |
| 13060 | DFT characterization on the effect of redox-inactive cation Ca ²⁺ on water oxidation by Coll-based cuboidal catalyst. <i>Computational and Theoretical Chemistry</i> , 2019, 1152, 1-6. | 1.1 | 0 |
| 13061 | Prediction of the Efficiency of Phosphorescent Emitters: A Theoretical Analysis of Triplet States in Platinum Blue Emitters. <i>Chemistry - A European Journal</i> , 2019, 25, 4202-4205. | 1.7 | 22 |
| 13062 | An Additivity Scheme for Aromaticity: The Heteroatom Case. <i>ChemPhysChem</i> , 2019, 20, 1508-1520. | 1.0 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 13063 | Scrutinizing the two new o-hydroxy Schiff bases from the point of tautomeric behavior and non-covalent interactions (H-bond, Br ⁻ ⋯Br, I ⁻ ⋯I ⁻ and C-H⋯I ⁻) in their supramolecular architectures. <i>Journal of Molecular Structure</i> , 2019, 1184, 427-434. | 1.8 | 12 |
| 13064 | Exciplex Stabilization in Asymmetric Acene Dimers. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1796-1806. | 1.1 | 13 |
| 13065 | Operators in quantum machine learning: Response properties in chemical space. <i>Journal of Chemical Physics</i> , 2019, 150, 064105. | 1.2 | 90 |
| 13066 | Dispersion Interaction and Crystal Packing Realize an Ultralong C-C Single Bond: A Theoretical Study on Dispirobis(10-methylacridan) Derivatives. <i>Chemistry Letters</i> , 2019, 48, 137-139. | 0.7 | 5 |
| 13067 | Reactivity of Gold(I) Monocarbene Complexes with Protein Targets: A Theoretical Study. <i>International Journal of Molecular Sciences</i> , 2019, 20, 820. | 1.8 | 34 |
| 13068 | Theoretical Insights Into Thermal Self-Initiation Reactions of Acrylates. , 2019, , 99-134. | | 1 |
| 13069 | High pressure Raman scattering of DL-isoleucine crystals and DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 214, 207-215. | 2.0 | 3 |
| 13070 | Thermodynamic and molecular insights into the absorption of H ₂ S, CO ₂ , and CH ₄ in choline chloride plus urea mixtures. <i>AIChE Journal</i> , 2019, 65, e16574. | 1.8 | 139 |
| 13071 | Sequential Cu-Catalyzed Four- and Five-Component Syntheses of Luminescent 3-Triazolylquinoxalines. <i>Chemistry - A European Journal</i> , 2019, 25, 9447-9455. | 1.7 | 13 |
| 13072 | Metal-metal interactions in binuclear cyclopentadienylmetal carbonyls: Extending insight from experimental work through computational studies. <i>Advances in Inorganic Chemistry</i> , 2019, , 3-32. | 0.4 | 4 |
| 13073 | Theoretical Studies on Hexanuclear [M ₃ (μ ₃ -O/OH)] ₂ (M = Fe(III), Tj ETQq0 0 0 rgBT /Overlock Correlations. <i>Inorganic Chemistry</i> , 2019, 58, 3175-3188. | 1.9 | 27 |
| 13074 | Self-Activated Coordination Polymerization of Alkoxystyrenes by a Yttrium Precursor: Stereocontrol and Mechanism. <i>ACS Catalysis</i> , 2019, 9, 2618-2625. | 5.5 | 40 |
| 13075 | Catalytic Enantioselective Hetero-[6+4] and -[6+2] Cycloadditions for the Construction of Condensed Polycyclic Pyrroles, Imidazoles, and Pyrazoles. <i>Journal of the American Chemical Society</i> , 2019, 141, 3288-3297. | 6.6 | 51 |
| 13076 | A high-rate and long-life organic oxygen battery. <i>Nature Materials</i> , 2019, 18, 390-396. | 13.3 | 110 |
| 13077 | Benchmarking quantum chemistry methods for spin-state energetics of iron complexes against quantitative experimental data. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4854-4870. | 1.3 | 99 |
| 13078 | Vacuum ultraviolet excited state dynamics of small amides. <i>Journal of Chemical Physics</i> , 2019, 150, 054301. | 1.2 | 7 |
| 13079 | Efficient HF exchange evaluation through Fourier convolution in Cartesian grid for orbital-dependent density functionals. <i>Journal of Chemical Physics</i> , 2019, 150, 064104. | 1.2 | 6 |
| 13080 | Accurate molecular polarizabilities with coupled cluster theory and machine learning. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 3401-3406. | 3.3 | 126 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13081 | Theoretical Surface Science Beyond Gradient-Corrected Density Functional Theory: Water at $\sqrt{2} \times \sqrt{3}$ (0001) as a Case Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6675-6684. | 1.5 | 15 |
| 13082 | Non-Aromatic 3-H-Pyrroles in the Reaction with Nucleophiles: Is High Reactivity a Myth?. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 2305-2312. | 1.2 | 6 |
| 13083 | Synthesis, characterization, computational and cytotoxic evaluation of novel [N, N-dialkyl ammonium] [diphenyl/ethyl phosphoryl oxides]. <i>Journal of Molecular Structure</i> , 2019, 1185, 183-190. | 1.8 | 5 |
| 13084 | Fingerprint of Aromaticity and Molecular Topology on the Photophysical Properties of Octaphyrins. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7318-7335. | 1.5 | 32 |
| 13085 | Investigation of the Electronic Structure of Aryl-Bridged Dinuclear U(III) and U(IV) Compounds. <i>Organometallics</i> , 2019, 38, 1031-1040. | 1.1 | 14 |
| 13086 | Self-Assembly of a Highly Emissive Pure Organic Imine-Based Stack for Electroluminescence and Cell Imaging. <i>Journal of the American Chemical Society</i> , 2019, 141, 4704-4710. | 6.6 | 101 |
| 13087 | Enantioselective Cu-catalyzed 1,4-additions of organozinc and Grignard reagents to enones: exceptional performance of the hydrido-phosphite-ligand BIFOP-H. <i>New Journal of Chemistry</i> , 2019, 43, 4787-4799. | 1.4 | 5 |
| 13088 | Bioactivity of a radical scavenger bis(pyrazolium <i>p</i> -toluenesulphonate) on ctDNA and certain microbes: a combined experimental and theoretical analysis. <i>Toxicology Research</i> , 2019, 8, 421-431. | 0.9 | 6 |
| 13089 | Deuterium isotope effect in fluorescence of gaseous oxazine dyes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5759-5770. | 1.3 | 24 |
| 13090 | Comparing the Self-Assembly of Sexiphenyl-Dicarbonitrile on Graphite and Graphene on Cu(111). <i>Chemistry - A European Journal</i> , 2019, 25, 5065-5070. | 1.7 | 4 |
| 13091 | The role of the halogen bond in iodothyronine deiodinase: Dependence on chalcogen substitution in naphthyl-based mimetics. <i>Journal of Computational Chemistry</i> , 2019, 40, 944-951. | 1.5 | 14 |
| 13092 | Equilibrium properties of protic ionic liquids based on methyl-2-hydroxyethylammonium cation. <i>Journal of Molecular Liquids</i> , 2019, 282, 226-234. | 2.3 | 3 |
| 13093 | Multiaim and Substituent Effects on Charge Transport of Organic Hole Transport Materials. <i>Chemistry of Materials</i> , 2019, 31, 6605-6614. | 3.2 | 21 |
| 13094 | Effect of the exchange correlation functional on the synchronicity/nonsynchronicity in bond formation in Diels-Alder reactions: a reaction force constant analysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7412-7428. | 1.3 | 31 |
| 13095 | A Trip to the Density Functional Theory Zoo: Warnings and Recommendations for the User. <i>Australian Journal of Chemistry</i> , 2019, 72, 563. | 0.5 | 115 |
| 13096 | Alkyne Activation with Gold(III) Complexes: A Quantitative Assessment of the Ligand Effect by Charge-Displacement Analysis. <i>Inorganic Chemistry</i> , 2019, 58, 3115-3129. | 1.9 | 18 |
| 13097 | A Nonheme Thiolate-Ligated Cobalt Superoxo Complex: Synthesis and Spectroscopic Characterization, Computational Studies, and Hydrogen Atom Abstraction Reactivity. <i>Journal of the American Chemical Society</i> , 2019, 141, 3641-3653. | 6.6 | 38 |
| 13098 | In Situ Measure of Intrinsic Bond Strength in Crystalline Structures: Local Vibrational Mode Theory for Periodic Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1761-1776. | 2.3 | 32 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13099 | Theoretical Study of Ruthenium(0)-Catalyzed Transfer Hydrogenative Cycloaddition of Cyclohexadiene and Norbornadiene with 1,2-Diols to Form Bridged Carbocycles. <i>Journal of Organic Chemistry</i> , 2019, 84, 3377-3387. | 1.7 | 3 |
| 13100 | Orbital-dependent redox potential regulation of quinone derivatives for electrical energy storage. <i>RSC Advances</i> , 2019, 9, 5164-5173. | 1.7 | 12 |
| 13101 | Competitive Inhibition of Quercetin and Apigenin at the ATP Binding site of D-Alanine-D-Alanine Ligase of <i>Helicobacter pylori</i> – A Molecular Modeling Approach. <i>Current Biotechnology</i> , 2019, 7, 340-348. | 0.2 | 5 |
| 13102 | Franck's Condon Blockade and Aggregation-Modulated Conductance in Molecular Devices Using Aggregation-Induced Emission-Active Molecules. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 5951-5955. | 7.2 | 36 |
| 13103 | Exploring the mechanism of alkene hydrogenation catalyzed by defined iron complex from DFT computation. <i>Journal of Molecular Modeling</i> , 2019, 25, 61. | 0.8 | 3 |
| 13104 | Accurate Prediction for Dynamic Hybrid Local and Charge Transfer Excited States from Optimally Tuned Range-Separated Density Functionals. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5616-5625. | 1.5 | 19 |
| 13105 | Aggregation control of Ru and Ir nanoparticles by tunable aryl alkyl imidazolium ionic liquids. <i>Nanoscale</i> , 2019, 11, 4073-4082. | 2.8 | 26 |
| 13106 | Elastic Properties of Lithium and Sodium Amides. <i>Russian Physics Journal</i> , 2019, 61, 1695-1701. | 0.2 | 2 |
| 13107 | Synthesis and characterization of a hydro tris(3-phenylpyrazolyl)borato nickel(II) semiquinonate adduct. <i>Polyhedron</i> , 2019, 162, 165-170. | 1.0 | 4 |
| 13108 | Recent Developments in Absolute Shielding Scales for NMR Spectroscopy. <i>Annual Reports on NMR Spectroscopy</i> , 2019, 96, 77-141. | 0.7 | 19 |
| 13109 | Chemical Insight on Decreased Sensitivity of CL-20/TNT Cocrystal Revealed by ReaxFF MD Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2079-2092. | 2.5 | 30 |
| 13110 | Impact of interfacial structure on the charge dynamics in nanocomposite dielectrics. <i>Journal of Applied Physics</i> , 2019, 125, 045109. | 1.1 | 6 |
| 13111 | Effect of Solvent Polarity on Bromobutyl Rubber Isomerization. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 2687-2693. | 0.1 | 1 |
| 13112 | A Computational Insight into Reaction Between Different Amino Acids with Reactive Aldehydes 4-hydroxy-2-nonenal and 4-oxo-2-nonenal. <i>Croatica Chemica Acta</i> , 2019, 92, 229-239. | 0.1 | 0 |
| 13113 | Threshold Dissociation of the 1-ethynylpyrene Cation at Internal Energies Relevant to H i Regions. <i>Astrophysical Journal</i> , 2019, 885, 21. | 1.6 | 4 |
| 13114 | Insulation Properties of Liquid C6F12O for the Use in Eco-Friendly Transmission Equipment. , 2019, , . | | 0 |
| 13115 | Formation and hydrolysis of gas-phase [UO ₂ (R)] ⁺ : R=CH ₃ , CH ₂ CH ₃ , CH ₂ CH ₂ CH ₃ , and C ₆ H ₅ . <i>Journal of Mass Spectrometry</i> , 2019, 54, 780-789. | 0.7 | 7 |
| 13116 | Dispersion-driven conformational preference in the gas phase: Microwave spectroscopic and theoretical study of allyl isocyanate. <i>Journal of Chemical Physics</i> , 2019, 151, 194304. | 1.2 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13117 | Four-component relativistic time-dependent density-functional theory using a stable noncollinear DFT ansatz applicable to both closed- and open-shell systems. <i>Journal of Chemical Physics</i> , 2019, 151, 184111. | 1.2 | 33 |
| 13118 | Some observations on the performance of the most recent exchange-correlation functionals for the large and chemically diverse GMTKN55 benchmark. <i>AIP Conference Proceedings</i> , 2019, , . | 0.3 | 15 |
| 13119 | Modeling of electronic and optical properties of C ₃ N ₄ within DFT frame. <i>AIP Conference Proceedings</i> , 2019, , . | 0.3 | 0 |
| 13120 | Straight, bendable and bent organic crystals. <i>Chemical Communications</i> , 2019, 55, 14749-14752. | 2.2 | 8 |
| 13121 | Stacking interactions of borazine: important stacking at large horizontal displacements and dihydrogen bonding governed by electrostatic potentials of borazine. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 24554-24564. | 1.3 | 5 |
| 13122 | Hyperfine tensors for a model system for the oxygen evolving complex of photosystem II: calculation of the anisotropy shift that occurs beyond the strong exchange limit. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22902-22909. | 1.3 | 2 |
| 13123 | The tetracapped truncated tetrahedron in 16-vertex tetrametallaborane structures: spherical aromaticity with an isocloso rather than a closo skeletal electron count. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22022-22030. | 1.3 | 5 |
| 13124 | The control effects of different scaffolds in chiral phosphoric acids: a case study of enantioselective asymmetric arylation. <i>Catalysis Science and Technology</i> , 2019, 9, 6482-6491. | 2.1 | 7 |
| 13125 | Localized high concentration electrolyte behavior near a lithium-metal anode surface. <i>Journal of Materials Chemistry A</i> , 2019, 7, 25047-25055. | 5.2 | 81 |
| 13126 | Isomer dependent molecular packing and carrier mobility of <i>N</i> -phenylcarbazole-phenanthro[9,10- <i>cd</i>]imidazole based materials as hosts for efficient electrophosphorescence devices. <i>Journal of Materials Chemistry C</i> , 2019, 7, 13486-13492. | 2.7 | 20 |
| 13127 | Structures and bonding properties of CPt ₂ O and CPt ₂ H ₂ O: Anion photoelectron spectroscopy and quantum chemical calculations. <i>Journal of Chemical Physics</i> , 2019, 151, 224303. | 1.2 | 7 |
| 13128 | Molecular Dynamics model of peptide-protein conjugation: case study of covalent complex between Sos1 peptide and N-terminal SH3 domain from Grb2. <i>Scientific Reports</i> , 2019, 9, 20219. | 1.6 | 3 |
| 13129 | Decomposition mechanism and kinetics of iso-C ₄ perfluoronitrile (C ₄ F ₇ N) plasmas. <i>Journal of Applied Physics</i> , 2019, 126, . | 1.1 | 20 |
| 13130 | Correlation effects in B _{1s} core-excited states of boronic-acid derivatives: An experimental and computational study. <i>Journal of Chemical Physics</i> , 2019, 151, 134306. | 1.2 | 4 |
| 13131 | Probing basis set requirements for calculating hyperfine coupling constants. <i>Journal of Chemical Physics</i> , 2019, 151, 174107. | 1.2 | 18 |
| 13132 | Accurate nuclear quadrupole moment of ruthenium from the molecular method. <i>Journal of Chemical Physics</i> , 2019, 151, 194306. | 1.2 | 1 |
| 13133 | Efficient calculation of NMR isotopic shifts: Difference-dedicated vibrational perturbation theory. <i>Journal of Chemical Physics</i> , 2019, 151, 244120. | 1.2 | 7 |
| 13134 | Computational study of regiodivergent pathways in the copper-catalyzed borocyanation of 1,3-dienes: Mechanism and origin of regioselectivity. <i>Journal of Organometallic Chemistry</i> , 2019, 904, 121014. | 0.8 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13135 | Functionalized Carbon Nanotube Excited States and Optical Properties. ACS Symposium Series, 2019, , 181-207. | 0.5 | 1 |
| 13136 | Template-free synthesis and metalation of hierarchical covalent organic framework spheres for photothermal therapy. Chemical Communications, 2019, 55, 14315-14318. | 2.2 | 34 |
| 13137 | BAR-based multi-dimensional nonequilibrium pulling for indirect construction of QM/MM free energy landscapes: from semi-empirical to <i>ab initio</i> . Physical Chemistry Chemical Physics, 2019, 21, 21942-21959. | 1.3 | 14 |
| 13138 | Structural peculiarities of keto-carotenoids in water-soluble proteins revealed by simulation of linear absorption. Physical Chemistry Chemical Physics, 2019, 21, 25707-25719. | 1.3 | 18 |
| 13139 | Comprehensive modelling study of singlet exciton diffusion in donor-acceptor dyads: when small changes in chemical structure matter. Physical Chemistry Chemical Physics, 2019, 21, 25023-25034. | 1.3 | 14 |
| 13140 | Trends of the macroscopic behaviors of energetic compounds: insights from first-principles calculations. Physical Chemistry Chemical Physics, 2019, 21, 24034-24041. | 1.3 | 3 |
| 13141 | Theoretical study of aromatic hydroxylation of the [Cu ₂ (H-XYL)O ₂] ²⁺ complex mediated by a side-on peroxo dicopper core and Cu-ligand effects. Dalton Transactions, 2019, 48, 16882-16893. | 1.6 | 1 |
| 13142 | Deciphering the mechanism of copper-catalyzed N-arylation between aryl halides and nitriles: a DFT study. New Journal of Chemistry, 2019, 43, 19200-19207. | 1.4 | 1 |
| 13143 | Activation reactions of 2-pyridyl and 2-pyrimidinyl alkynes with Ru ₃ (CO) ₁₂ . New Journal of Chemistry, 2019, 43, 19075-19084. | 1.4 | 1 |
| 13144 | Screening the 4f-electron spin of TbPc ₂ single-molecule magnets on metal substrates by ligand channeling. Nanoscale, 2019, 11, 21167-21179. | 2.8 | 17 |
| 13145 | Origins of stereoselectivity in uncatalyzed and ZnBr ₂ -catalyzed Diels-Alder reactions of a chiral sulfinylquinone. Organic and Biomolecular Chemistry, 2019, 17, 8756-8767. | 1.5 | 0 |
| 13146 | Chiral Selectivity in the Achiral Amino Acid Glycine. Journal of Organic Chemistry, 2019, 84, 16199-16203. | 1.7 | 6 |
| 13147 | Conformational Equilibria and Molecular Structures of Model Sulfur-Sulfur Bridge Systems: Diisopropyl Disulfide. Journal of Physical Chemistry A, 2019, 123, 10714-10720. | 1.1 | 5 |
| 13148 | Decomposition characteristics of C ₄ F ₇ N/CO ₂ mixture under AC discharge breakdown. AIP Advances, 2019, 9, . | 0.6 | 40 |
| 13149 | Quantum-Chemical Study of Adsorption of Tl ⁺ Ions on Au(111). Russian Journal of Electrochemistry, 2019, 55, 1009-1020. | 0.3 | 0 |
| 13150 | Computational Characterization of Perezone, Isoperezone and their Sulfur-Derivatives: Anti-Inflammatory Activity.. ChemistrySelect, 2019, 4, 13333-13346. | 0.7 | 6 |
| 13151 | Modeling chemical reactions on surfaces: The roles of chemical bonding and van der Waals interactions. Progress in Surface Science, 2019, 94, 100561. | 3.8 | 39 |
| 13152 | Evolution of Magnetic Anisotropy of an Organometallic Molecule in a Mechanically Controlled Break Junction: The Roles of Connecting Electrodes. Journal of Physical Chemistry C, 2019, 123, 30754-30764. | 1.5 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13153 | Synthesis of (±)-cis-1-Aryl-3-oxo-2,3-dihydro-1H-benzo[f]chromene-2-carbonitriles and (±)-trans-1,4-Aryl-2-oxo-3,4-dihydro-2H-benzo[h]chromene-3-carbonitriles. <i>ChemistrySelect</i> , 2019, 4, 12902-12905. Excitons in InP, GaP, and GaAs | | 1 |
| 13154 | GaInP quantum dots: Insights from time-dependent density functional theory. <i>Physical Review B</i> , 2019, 100, ... | 1.1 | 8 |
| 13155 | Few-Layered Fluorinated Triazine-Based Covalent Organic Nanosheets for High-Performance Alkali Organic Batteries. <i>ACS Nano</i> , 2019, 13, 14252-14261. | 7.3 | 158 |
| 13156 | Synthesis and Structures of 1,3-Dicarbonyl Compounds Based on 9,10-Phenanthrenequinone. Crystal and Molecular Structure of the Lantern-Type Binuclear Copper(II) Complex $\text{Cu}_2[\text{1/4-2-OOCCH}_2(\text{C}_{14}\text{H}_8)(\text{CO})_2\text{OC}_2\text{H}_5]_4(\text{NCCH}_3)_2$. <i>Crystallography Reports</i> , 2019, 64, 887-893. | 0.1 | 0 |
| 13157 | Comparison of Experimental and Experimental-Theoretical Topological Characteristics of the Electron Density in the Crystalline Complex $\text{[6-[3-Acetyl-tetrahydro-6-Phenyl-2H-1,3-oxazine]tricarboxylchromium(0)}$. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2019, 45, 680-688. | 0.3 | 9 |
| 13158 | Synthesis and Antimicrobial Activity of N-(Indolyl)trifluoroacetamides. <i>Moscow University Chemistry Bulletin</i> , 2019, 74, 236-240. | 0.2 | 4 |
| 13159 | (3S,4R)-3,4-Dihydroxy-N-alkyl-L-homoprolines: synthesis and computational mechanistic studies. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 10052-10064. | 1.5 | 1 |
| 13160 | Excess electron solvation in ammonia clusters. <i>Journal of Chemical Physics</i> , 2019, 151, 204304. | 1.2 | 13 |
| 13161 | Radical Stabilization Energies for Enzyme Engineering: Tackling the Substrate Scope of the Radical Enzyme QueE. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 5111-5125. | 2.5 | 7 |
| 13162 | Guanidinocalix[5]arene for sensitive fluorescence detection and magnetic removal of perfluorinated pollutants. <i>Nature Communications</i> , 2019, 10, 5762. | 5.8 | 116 |
| 13163 | Fiber-Array-Based Raman Hyperspectral Imaging for Simultaneous, Chemically-Selective Monitoring of Particle Size and Shape of Active Ingredients in Analgesic Tablets. <i>Molecules</i> , 2019, 24, 4381. | 1.7 | 22 |
| 13164 | Highly Sensitive Detection of the Antibiotic Ciprofloxacin by Means of Fiber Enhanced Raman Spectroscopy. <i>Molecules</i> , 2019, 24, 4512. | 1.7 | 20 |
| 13165 | DFT Modeling of Organocatalytic Ring-Opening Polymerization of Cyclic Esters: A Crucial Role of Proton Exchange and Hydrogen Bonding. <i>Polymers</i> , 2019, 11, 2078. | 2.0 | 23 |
| 13166 | A Novel Design Strategy for Suppressing Efficiency Roll-Off of Blue Thermally Activated Delayed Fluorescence Molecules through Donor-Acceptor Interlocking by C-C Bonds. <i>Nanomaterials</i> , 2019, 9, 1735. | 1.9 | 7 |
| 13167 | The allosteric mechanism of substrate-specific transport in SLC6 is mediated by a volumetric sensor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 15947-15956. | 3.3 | 23 |
| 13168 | Unraveling the Multi-Enzyme-Like Activities of Iron Oxide Nanozyme via a First-Principles Microkinetic Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 30318-30334. | 1.5 | 42 |
| 13169 | Correlation between the pKa and nuclear shielding of β -hydrogen of ketones. <i>Journal of Molecular Modeling</i> , 2019, 25, 354. | 0.8 | 3 |
| 13170 | Fluoreno[2,1-a]fluorene: an ortho-naphthoquinodimethane-based system with partial diradical character. <i>Chemical Communications</i> , 2019, 55, 14186-14189. | 2.2 | 15 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13171 | Insight into the structure and bonding of copper(i) iodide clusters and a cluster-based coordination polymer. <i>New Journal of Chemistry</i> , 2019, 43, 16176-16187. | 1.4 | 4 |
| 13172 | Electronic effects in tautomeric equilibria: the case of chiral imines from <scpd>-glucamine and 2-hydroxyacetophenones. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 10209-10222. | 1.5 | 5 |
| 13173 | Development of a quantum chemical descriptor expressing aromatic/quinoidal character for designing narrow-bandgap π -conjugated polymers. <i>Polymer Chemistry</i> , 2019, 10, 5584-5593. | 1.9 | 12 |
| 13174 | New synthesis of tetraoxaspirododecane-diamines and tetraoxazaspirobicycloalkanes. <i>RSC Advances</i> , 2019, 9, 29949-29958. | 1.7 | 14 |
| 13175 | A collection of forcefield precursors for metal-organic frameworks. <i>RSC Advances</i> , 2019, 9, 36492-36507. | 1.7 | 21 |
| 13176 | A model for dinitrogen binding in the E ₄ state of nitrogenase. <i>Chemical Science</i> , 2019, 10, 11110-11124. | 3.7 | 48 |
| 13177 | Does the length matter? - Synthesis, photophysical, and theoretical study of novel quinolines based on carbazoles with different length of alkyl chain. <i>Dyes and Pigments</i> , 2019, 160, 604-613. | 2.0 | 28 |
| 13178 | Ethene-bridged diiron porphyrin dimer as models of diheme cytochrome c: Structure-function correlation and modulation of heme redox potential. <i>Inorganica Chimica Acta</i> , 2019, 484, 503-512. | 1.2 | 15 |
| 13179 | Energy bandgap engineering of graphene nanoribbon by doping phosphorous impurities to create nano-heterostructures: A DFT study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019, 105, 105-115. | 1.3 | 15 |
| 13180 | Structure and redox properties of polymethine dyes: Electrochemical and DFT/TD-DFT study. <i>Dyes and Pigments</i> , 2019, 161, 24-33. | 2.0 | 25 |
| 13181 | Ln-Pt electron polarization effects on the magnetic relaxation of heterometallic Ho and Er complexes. <i>Dalton Transactions</i> , 2019, 48, 7144-7149. | 1.6 | 10 |
| 13182 | Excited-State Reactivity of [Mn(im)(CO) ₃ (phen)] ⁺ : A Structural Exploration. <i>Journal of Computational Chemistry</i> , 2019, 40, 72-81. | 1.5 | 7 |
| 13183 | Structural Characterization of Molybdenum Oxide Nanoclusters Using Ion Mobility Spectrometry-Mass Spectrometry and Infrared Action Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7845-7853. | 1.5 | 20 |
| 13184 | Quantum Monte Carlo assessment of density functionals for π -electron molecules: ethylene and bifuran. <i>Molecular Physics</i> , 2019, 117, 2241-2250. | 0.8 | 1 |
| 13185 | The Role of the Fluoro-Hydrido-Phosphorane Intermediate in Catalytic Hydrosilylation of Acetophenone: Computational Study. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 318-322. | 1.2 | 6 |
| 13186 | Synthesis, characterization, and theoretical studies of (E)-t-butyl-2-((E)-2-methyl-3-phenylallylidene) hydrazine carboxylate and (E)-t-butyl-2-((E)-3-phenylallylidene) hydrazine carboxylates as a possible Mcl-1 antagonists. <i>Journal of Molecular Structure</i> , 2019, 1181, 197-202. | 1.8 | 6 |
| 13187 | Imaging electron-density fluctuations by multidimensional X-ray photon-coincidence diffraction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 395-400. | 3.3 | 4 |
| 13188 | Employing broken symmetry effects from unrestricted coupled cluster wave function to determine dynamic and non-dynamic electron correlation during triple bond breaking in the N ₂ molecule. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25865. | 1.0 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13189 | Theisoclosocapped pentagonal bipyramid versus the closobisdisphenoid in hypoelectronic eight-vertex metallaboranes having 16 skeletal electrons. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25880. | 1.0 | 0 |
| 13190 | Atmospheric \hat{I}^2 -Caryophyllene-Derived Ozonolysis Products at Interfaces. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 158-169. | 1.2 | 10 |
| 13191 | Density matrix renormalization group pair-density functional theory (DMRG-PDFT): singlet-triplet gaps in polyacenes and polyacetylenes. <i>Chemical Science</i> , 2019, 10, 1716-1723. | 3.7 | 69 |
| 13192 | Highly efficient adsorption of benzothiophene from model fuel on a metal-organic framework modified with dodeca-tungstophosphoric acid. <i>Chemical Engineering Journal</i> , 2019, 362, 30-40. | 6.6 | 28 |
| 13193 | Syntheses and Structures of a Series of Acyclic Diaminocarbene Palladium(II) Complexes Derived from 3,4-Diaryl-1 <i>H</i> -pyrrol-2,5-diimines and Bisocyanide Palladium(II) Complexes. <i>Organometallics</i> , 2019, 38, 300-309. | 1.1 | 11 |
| 13194 | Benson group additivity values of phosphines and phosphine oxides: Fast and accurate computational thermochemistry of organophosphorus species. <i>Journal of Computational Chemistry</i> , 2019, 40, 572-580. | 1.5 | 4 |
| 13195 | Halogen and Chalcogen Binding Dominated by Density-Driven Errors. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 295-301. | 2.1 | 43 |
| 13196 | More than Expected: Overall Initiation Efficiencies of Mono-, Bis-, and Tetraacylgermane Radical Initiators. <i>Macromolecules</i> , 2019, 52, 281-291. | 2.2 | 19 |
| 13197 | Tropylium and Porphyrinoid Character in Carbaporphyrinoid Systems. Relative Stability and Aromatic Characteristics of Azuliporphyrin and Tropiporphyrin Tautomers, Protonated Species, and Related Structures. <i>Journal of Physical Chemistry A</i> , 2019, 123, 230-246. | 1.1 | 13 |
| 13198 | Photocatalytic Hydrogen Evolution from Water Using Fluorene and Dibenzothiophene Sulfone-Conjugated Microporous and Linear Polymers. <i>Chemistry of Materials</i> , 2019, 31, 305-313. | 3.2 | 173 |
| 13199 | Method for Simultaneous Prediction of Atomic Structure and Stability of Nanoclusters in a Wide Area of Compositions. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 102-106. | 2.1 | 34 |
| 13200 | Synthesis of Amidines by Palladium-Mediated CO ₂ Extrusion Followed by Insertion of Carbodiimides: Translating Mechanistic Studies to Develop a One-Pot Method. <i>Organometallics</i> , 2019, 38, 424-435. | 1.1 | 16 |
| 13201 | What Are the Radical Intermediates in Oxidative <i>N</i> -Heterocyclic Carbene Organocatalysis?. <i>Journal of the American Chemical Society</i> , 2019, 141, 1109-1117. | 6.6 | 88 |
| 13202 | Alkyne Versus Ynamide Reactivity: Regioselective Radical Cyclization of γ -Ynamides. <i>Angewandte Chemie</i> , 2019, 131, 2311-2316. | 1.6 | 11 |
| 13203 | Computational investigation into the fluorescence of luciferin analogues. <i>Journal of Computational Chemistry</i> , 2019, 40, 527-531. | 1.5 | 7 |
| 13204 | An experimental and computational approach to pH-dependent self-assembly of poly(2-isopropyl-2-oxazoline). <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2019, 57, 210-221. | 2.4 | 7 |
| 13205 | Synthesis of Camphor-Derived Bis(pyrazolylpyridine) Rhodium(III) Complexes: Structure-Reactivity Relationships and Biological Activity. <i>Inorganic Chemistry</i> , 2019, 58, 307-319. | 1.9 | 28 |
| 13206 | β -Facial Selectivities in Hydride Reductions of Hindered Endocyclic Iminium Ions. <i>Journal of Organic Chemistry</i> , 2019, 84, 273-281. | 1.7 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13207 | Development of New Epoxy Resin Monomers – A Delicate Balance between Skin Allergy and Polymerization Properties. <i>Chemical Research in Toxicology</i> , 2019, 32, 57-66. | 1.7 | 7 |
| 13208 | Alkyne Versus Ynamide Reactivity: Regioselective Radical Cyclization of Yne–Ynamides. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 2289-2294. | 7.2 | 69 |
| 13209 | Isolation of the Metalated Ylides $[Ph_3P^+C^{\ominus}CN]M$ (M=Li, Na, K): Influence of the Metal Ion on the Structure and Bonding Situation. <i>Chemistry - A European Journal</i> , 2019, 25, 2793-2802. | 1.7 | 17 |
| 13210 | High level ab initio thermochemistry of SF5OOO radical. <i>Computational and Theoretical Chemistry</i> , 2019, 1148, 8-15. | 1.1 | 2 |
| 13211 | Tri- and tetranuclear heteropivalate complexes with core $\{Fe_2NiO\}$ ($\chi^{\ominus} = \ominus 1, 2$): Synthesis, structure, magnetic and thermal properties. <i>Polyhedron</i> , 2019, 159, 426-435. | 1.0 | 20 |
| 13212 | Toward Building Protein Force Fields by Residue-Based Systematic Molecular Fragmentation and Neural Network. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1409-1417. | 2.3 | 18 |
| 13213 | Synthesis and Luminescence Properties of Near-Infrared <i>N</i> -Heterocyclic Luciferin Analogues for <i>In Vivo</i> Optical Imaging. <i>Bulletin of the Chemical Society of Japan</i> , 2019, 92, 608-618. | 2.0 | 21 |
| 13214 | Gas phase fragmentation of adducts between dioxygen and closo-borate radical anions. <i>International Journal of Mass Spectrometry</i> , 2019, 436, 71-78. | 0.7 | 5 |
| 13215 | Structural, photophysical and electrochemical properties of a novel cardanol-based salophen ligand and its Mn(II) complex. <i>Journal of Molecular Structure</i> , 2019, 1181, 279-286. | 1.8 | 8 |
| 13216 | Identification performance of two luminescent lanthanide–organic frameworks. <i>Polyhedron</i> , 2019, 161, 40-46. | 1.0 | 7 |
| 13217 | Design, two-directional synthesis, DFT study of new pyrimido[5,4-d]pyrimidine-2,8-dione derivatives. <i>Tetrahedron</i> , 2019, 75, 749-756. | 1.0 | 7 |
| 13218 | Hydrogen-Bond-Dependent Conformational Switching: A Computational Challenge from Experimental Thermochemistry. <i>Journal of Organic Chemistry</i> , 2019, 84, 613-621. | 1.7 | 5 |
| 13219 | Photophysics of OLED Materials with Emitters Exhibiting Thermally Activated Delayed Fluorescence and Used in Hole/Electron Transporting Layer from Optimally Tuned Range-Separated Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2019, 123, 746-761. | 1.5 | 18 |
| 13220 | DFT Studies on the Mechanism of Copper-Catalyzed Boracarboxylation of Alkene with CO_2 and Diboron. <i>Organometallics</i> , 2019, 38, 240-247. | 1.1 | 36 |
| 13221 | Van der Waals effects on structure and optical properties in organic photovoltaics. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25883. | 1.0 | 8 |
| 13222 | Kinetic Resolution of Alkylidene Norcamphors via a Ligand-Controlled Umpolung-Type 1,3-Dipolar Cycloaddition. <i>IScience</i> , 2019, 11, 146-159. | 1.9 | 25 |
| 13223 | A GROMOS Force Field for Furanose-Based Carbohydrates. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1168-1186. | 2.3 | 31 |
| 13224 | Germanium Fluoride Nanocages as Optically Transparent n-Type Materials and Their Endohedral Metallofullerene Derivatives. <i>Journal of the American Chemical Society</i> , 2019, 141, 1672-1684. | 6.6 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13225 | Doubly Nâ€Confused Calix[6]phyrin Bisâ€Organopalladium Complexes: Photostable Triplet Sensitizers for Singlet Oxygen Generation. <i>Chemistry - an Asian Journal</i> , 2019, 14, 1729-1736. | 1.7 | 14 |
| 13226 | Towards the Design of Optically Active Thiophene Sâ€Oxides using Quantum Chemistry. <i>Chemistry - A European Journal</i> , 2019, 25, 2840-2851. | 1.7 | 2 |
| 13227 | Evaluating Computational and Structural Approaches to Predict Transformation Products of Polycyclic Aromatic Hydrocarbons. <i>Environmental Science & Technology</i> , 2019, 53, 1595-1607. | 4.6 | 15 |
| 13228 | Enantioselective Electrophilic Aromatic Nitration: A Chiral Auxiliary Approach. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 1035-1040. | 7.2 | 19 |
| 13229 | Solvent effects on the vibrational spectrum of 3-hydroxyflavone. <i>Journal of Molecular Liquids</i> , 2019, 275, 723-728. | 2.3 | 10 |
| 13230 | Theoretical study on the base-controlled selective linear or branched ortho-alkylation of azines catalyzed by rhodium: Mechanisms and the role of base. <i>Molecular Catalysis</i> , 2019, 462, 77-84. | 1.0 | 9 |
| 13231 | Push it to the limit: comparing periodic and local approaches to density functional theory for intermolecular interactions. <i>Molecular Physics</i> , 2019, 117, 1298-1305. | 0.8 | 6 |
| 13232 | Development of Divide&Conquer Densityâ€Functional Tightâ€Binding Method for Theoretical Research on Liâ€Ion Battery. <i>Chemical Record</i> , 2019, 19, 746-757. | 2.9 | 15 |
| 13233 | Design, synthesis and QSAR study of 2â€-hydroxy-4â€-alkoxy chalcone derivatives that exert cytotoxic activity by the mitochondrial apoptotic pathway. <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 43-54. | 1.4 | 28 |
| 13234 | N-methylation versus oxidative addition using MeI in the reaction of organoplatinum(II) complexes containing pyrazine ligand. <i>Journal of Organometallic Chemistry</i> , 2019, 880, 232-240. | 0.8 | 5 |
| 13235 | Enantioselective Electrophilic Aromatic Nitration: A Chiral Auxiliary Approach. <i>Angewandte Chemie</i> , 2019, 131, 1047-1052. | 1.6 | 8 |
| 13236 | The nature of photoinduced intermolecular charger transfer in fluorescence resonance energy transfer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 209, 228-233. | 2.0 | 19 |
| 13237 | A High-Capacity, Reversible Liquid Organic Hydrogen Carrier: H ₂ -Release Properties and an Application to a Fuel Cell. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 1185-1194. | 3.2 | 55 |
| 13238 | Novel rhodium on carbon catalysts for the oxidation of benzyl alcohol to benzaldehyde: A study of the modification of metal/support interactions by acid pre-treatments. <i>Applied Catalysis A: General</i> , 2019, 570, 271-282. | 2.2 | 18 |
| 13239 | Aldol Condensation Reaction of Methyl Acetate and Formaldehyde Over Cesium Oxide Supported on Silica Gel: An Experimental and Theoretical Study. <i>Catalysis Letters</i> , 2019, 149, 373-389. | 1.4 | 21 |
| 13240 | Hybrid-DFT Modeling of Lattice and Surface Vacancies in MnO. <i>Journal of Physical Chemistry C</i> , 2019, 123, 8133-8144. | 1.5 | 10 |
| 13241 | Photoalignmentability of silsesquioxane-containing citraconimide and its solvent-induced surface enrichment in PMMA matrix. <i>Liquid Crystals</i> , 2019, 46, 884-895. | 0.9 | 1 |
| 13242 | Origins of chemoselectivity of Rh(III)-Catalyzed Câ€H activation of N-(pivaloyloxy)benzamide: Insights from density functional theory calculations. <i>Journal of Organometallic Chemistry</i> , 2019, 880, 163-169. | 0.8 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13243 | Urban Particulate Matter-Induced Decomposition of <i>S</i> -Nitrosoglutathione Relevant to Aberrant Nitric Oxide Biological Signaling. <i>ChemSusChem</i> , 2019, 12, 661-671. | 3.6 | 7 |
| 13244 | Combined spectroscopic, molecular docking and quantum mechanics study of β -casein and ferulic acid interactions following UHT-like treatment. <i>Food Hydrocolloids</i> , 2019, 89, 351-359. | 5.6 | 50 |
| 13245 | A family of solution processable ligands and their Re(I) complexes towards light emitting applications. <i>Dyes and Pigments</i> , 2019, 163, 86-101. | 2.0 | 22 |
| 13246 | A molecular modelling study of the effects of pivalate ligand substitutions on the magnetic properties of chromium-wheels host complexes. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 87, 41-47. | 1.3 | 1 |
| 13247 | Nitrogen hybridization controls peroxo-oxo equilibrium in ethylenediamine bound binuclear [Cu ₂ O ₂] complexes. <i>Inorganica Chimica Acta</i> , 2019, 487, 63-69. | 1.2 | 1 |
| 13248 | Effect of Coordination Modes on the Tunable Luminescence of 1,10-Phenanthroline-Based Complexes. <i>Crystal Research and Technology</i> , 2019, 54, 1800168. | 0.6 | 1 |
| 13249 | On the Stability of Disubstituted Cyclobutenes – A Computational Study. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 338-341. | 1.2 | 7 |
| 13250 | Decomposition of Piloty's acid derivatives – Toward the understanding of factors controlling HNO release. <i>Archives of Biochemistry and Biophysics</i> , 2019, 661, 132-144. | 1.4 | 11 |
| 13251 | Effective redox reactions by chromium oxide anions: Sulfur dioxide oxidation in the gas phase. <i>International Journal of Mass Spectrometry</i> , 2019, 436, 18-22. | 0.7 | 10 |
| 13252 | An ONIOM investigation of the effect of conformation on bond dissociation energies in peptides. <i>Journal of Computational Chemistry</i> , 2019, 40, 82-88. | 1.5 | 6 |
| 13253 | Synthesis and Characterization of Oxazaborinin Phosphonate for Blue OLED Emitter Applications. <i>ChemPhysChem</i> , 2019, 20, 665-671. | 1.0 | 7 |
| 13254 | 1,2,3-Propanetriol radicals formed during oxidative stress. <i>Magnetic Resonance in Chemistry</i> , 2019, 57, S95-S100. | 1.1 | 0 |
| 13255 | Elucidating the Nuclear Quantum Dynamics of Intramolecular Double Hydrogen Transfer in Porphycene. <i>Journal of the American Chemical Society</i> , 2019, 141, 2526-2534. | 6.6 | 68 |
| 13256 | Synthesis of Cyclobutane-Fused Angular Tetracyclic Spiroindolines via Visible-Light-Promoted Intramolecular Dearomatization of Indole Derivatives. <i>Journal of the American Chemical Society</i> , 2019, 141, 2636-2644. | 6.6 | 177 |
| 13257 | Structures and binding energies for complexations of different spin states of Ni ⁺ and Ni ²⁺ to aromatic molecules. <i>Molecular Physics</i> , 2019, 117, 1392-1403. | 0.8 | 4 |
| 13258 | A problem in the structure assignment of acremolin C, which is most probably identical with acremolin B. <i>Natural Product Research</i> , 2019, 33, 3011-3015. | 1.0 | 5 |
| 13259 | Fabrication of new metal-free materials for the hydrogen evolution reaction on base of the acridine derivatives immobilized on carbon materials. <i>Materials Chemistry and Physics</i> , 2019, 224, 148-155. | 2.0 | 12 |
| 13260 | Thermal decomposition of bimetallic titanium complexes: A new method for synthesizing doped titanium nano-sized catalysts and photocatalytic application. <i>Materials Science and Engineering C</i> , 2019, 97, 813-826. | 3.8 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13261 | Fast and Accurate Uncertainty Estimation in Chemical Machine Learning. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 906-915. | 2.3 | 102 |
| 13262 | Coll Complexes with a Tripyridine Ligand, Containing a 2,6-Di-tert-butylphenolic Fragment: Synthesis, Structure, and Formation of Stable Radicals. <i>ACS Omega</i> , 2019, 4, 203-213. | 1.6 | 3 |
| 13263 | Metatox - Web application for generation of metabolic pathways and toxicity estimation. <i>Journal of Bioinformatics and Computational Biology</i> , 2019, 17, 1940001. | 0.3 | 13 |
| 13264 | A mild and efficient procedure for alkenols oxyselenocyclization by using ionic liquids. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3928. | 0.9 | 5 |
| 13265 | Synthesis and Properties of Novel Fluorescence Probe Based on 1,8-Naphthalimide for Detection of Hydrogen Sulfide. <i>Chemical Research in Chinese Universities</i> , 2019, 35, 5-11. | 1.3 | 13 |
| 13266 | Structure, stability and conversions of tautomers and rotamers of azulene-based uracil analogue. <i>Journal of Molecular Structure</i> , 2019, 1182, 271-282. | 1.8 | 7 |
| 13267 | The Curious Case of Acetaldehyde Phenylhydrazone: Resolution of a 120 Year Old Puzzle where Forms with Vastly Different Melting Points Have the Same Structure. <i>Crystal Growth and Design</i> , 2019, 19, 907-917. | 1.4 | 7 |
| 13268 | Aza-Nazarov Cyclization Reactions via Anion Exchange Catalysis. <i>Organic Letters</i> , 2019, 21, 554-558. | 2.4 | 11 |
| 13269 | Solvent effects on the absorption and fluorescence spectra of Zaleplon: Determination of ground and excited state dipole moments. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 212, 356-362. | 2.0 | 24 |
| 13270 | Unraveling Anhydrous Proton Conduction in Hydroxygraphane. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 518-523. | 2.1 | 13 |
| 13271 | Charge-state analysis of small barium-oxide clusters by x-ray absorption spectroscopy. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 134003. | 0.7 | 2 |
| 13272 | The electronic complexity of the ground-state of the FeMo cofactor of nitrogenase as relevant to quantum simulations. <i>Journal of Chemical Physics</i> , 2019, 150, 024302. | 1.2 | 59 |
| 13273 | Complexes formed by the siderophore-based monosulfactam antibiotic BAL30072 and their interaction with the outer membrane receptor PiuA of <i>P. aeruginosa</i> . <i>BioMetals</i> , 2019, 32, 155-170. | 1.8 | 8 |
| 13274 | Prediction of ion selectivity by quantum chemical calculations X: A recent (personal) review. <i>Advances in Inorganic Chemistry</i> , 2019, 73, 445-505. | 0.4 | 9 |
| 13275 | Homolytic S Cl bond dissociation enthalpies of sulfenyl chlorides – a high-level G4 thermochemical study. <i>Chemical Data Collections</i> , 2019, 19, 100180. | 1.1 | 3 |
| 13276 | Palladium(II) complexes containing seven halogeno-derivatives of 7-azaindole: molecular structures, vibrational spectra, DFT calculations and in vitro cytotoxic activity. <i>Journal of Molecular Structure</i> , 2019, 1181, 444-454. | 1.8 | 6 |
| 13277 | New heteroleptic iridium(III) nitro complexes derived from fac-[Ir(NO ₂) ₃ (H ₂ O) ₃]. <i>Journal of Molecular Structure</i> , 2019, 1182, 100-108. | 1.8 | 3 |
| 13278 | A study of the optical, electrical and structural properties of poly(pyrrole-3,4-dicarboxylic acid). <i>Polymer</i> , 2019, 164, 142-153. | 1.8 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13279 | Competitive Intramolecular Amination as a Clock for Iron-Catalyzed Nitrene Transfer. <i>Inorganic Chemistry</i> , 2019, 58, 1107-1119. | 1.9 | 7 |
| 13280 | NMR Shielding Tensors and Chemical Shifts in Scalar-Relativistic Local Exact Two-Component Theory. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1028-1043. | 2.3 | 46 |
| 13281 | Proton Affinities of N-Heterocyclic Olefins and Their Implications for Organocatalyst Design. <i>Journal of Organic Chemistry</i> , 2019, 84, 2209-2218. | 1.7 | 36 |
| 13282 | Borepin Rings as σ -Free Reporters of Aromaticity within Polycyclic Aromatic Scaffolds. <i>Journal of Physical Chemistry A</i> , 2019, 123, 881-888. | 1.1 | 10 |
| 13283 | Probing Surface Chemistry at an Atomic Level: Decomposition of 1-Propanethiol on GaP(001) (2 Å–4) Investigated by STM, XPS, and DFT. <i>Journal of Physical Chemistry C</i> , 2019, 123, 2964-2972. | 1.5 | 0 |
| 13284 | Evidence for Hidden Involvement of N3-Protonated Guanine in RNA Structure and Function. <i>ACS Omega</i> , 2019, 4, 699-709. | 1.6 | 8 |
| 13285 | Asymmetric Transfer Hydrogenation with a Bifunctional Iron(II) Hydride: Experiment Meets Computation. <i>Journal of the American Chemical Society</i> , 2019, 141, 2545-2556. | 6.6 | 39 |
| 13286 | Magnetic moments of small cobalt clusters revisited: The contribution of 3d and 4s electrons. <i>International Journal of Mass Spectrometry</i> , 2019, 438, 135-141. | 0.7 | 1 |
| 13287 | Magnetic Cationic Copper(II) Chains and a Mononuclear Cobalt(II) Complex Containing [Ln(hfac) ₄] ⁺ Blocks as Counterions. <i>Inorganic Chemistry</i> , 2019, 58, 1976-1987. | 1.9 | 18 |
| 13288 | Systematic Assessment of Benzenethiol Self-Assembled Monolayers on Au(111) as a Standard Sample for Electrochemical Tip-Enhanced Raman Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2019, 123, 2953-2963. | 1.5 | 30 |
| 13289 | Discovery of High Affinity Receptors for Dityrosine through Inverse Virtual Screening and Docking and Molecular Dynamics. <i>International Journal of Molecular Sciences</i> , 2019, 20, 115. | 1.8 | 24 |
| 13290 | Electrochemical and electronic properties of a series of substituted polypyridine ligands and their Co(II) complexes. <i>Inorganica Chimica Acta</i> , 2019, 486, 26-35. | 1.2 | 26 |
| 13291 | Rate constants of C ₅ F ₁₀ O decomposition reactions at temperatures of 300–3500 K. <i>Journal Physics D: Applied Physics</i> , 2019, 52, 035202. | 1.3 | 27 |
| 13292 | Stereochemical assignment of four diastereoisomers of a maculactone derivative by computational NMR calculations. <i>Journal of Molecular Structure</i> , 2019, 1178, 467-478. | 1.8 | 3 |
| 13293 | Puzzling Reaction of Imidazole with Methyl Parathion: P=S versus P=O Mechanistic Shift Dilemma in Organophosphates. <i>Chemistry - A European Journal</i> , 2019, 25, 817-822. | 1.7 | 11 |
| 13294 | Renewable-lawsone-based sustainable and high-voltage aqueous flow battery. <i>Energy Storage Materials</i> , 2019, 19, 62-68. | 9.5 | 30 |
| 13295 | Phloroglucinols from the Roots of <i>Garcinia dauphinensis</i> and Their Antiproliferative and Antiplasmodial Activities. <i>Journal of Natural Products</i> , 2019, 82, 431-439. | 1.5 | 16 |
| 13296 | Spin–spin coupling constants in linear substituted HCN clusters. <i>Molecular Physics</i> , 2019, 117, 693-704. | 0.8 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 13297 | Multireference exciplex binding energies: Basis set convergence and error. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25819. | 1.0 | 8 |
| 13298 | Accurate heats of formation of polycyclic saturated hydrocarbons predicted by using the XYG3 type of doubly hybrid functionals. <i>Journal of Computational Chemistry</i> , 2019, 40, 1113-1122. | 1.5 | 6 |
| 13299 | 2-Amino-4-(4-methoxyphenyl)-thiazole as a novel corrosion inhibitor for mild steel in acidic medium. <i>Progress in Organic Coatings</i> , 2019, 126, 150-161. | 1.9 | 61 |
| 13300 | Revealing Photoluminescence Modulation from Layered Halide Perovskite Microcrystals upon Cyclic Compression. <i>Advanced Materials</i> , 2019, 31, e1805608. | 11.1 | 16 |
| 13301 | InÂvitro and in silico studies of antioxidant activity of 2-thiazolylhydrazone derivatives. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 86, 106-112. | 1.3 | 13 |
| 13302 | Excited state hydrogen atom transfer in micro-solvated dicoumarol: A TDDFT/EFP1 study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 208, 325-330. | 2.0 | 1 |
| 13303 | Gas phase basicity of biguanides â€“ Comparison of the equilibrium and the kinetic methods. <i>International Journal of Mass Spectrometry</i> , 2019, 435, 61-68. | 0.7 | 9 |
| 13304 | Vibrational Spectroscopy in Analysis of Stimuli-Responsive Polymerâ€™Water Systems. Challenges and Advances in Computational Chemistry and Physics, 2019, , 223-271. | 0.6 | 0 |
| 13305 | New mechanistic insights into the Claisen rearrangement of chorismate â€“ a Unified Reaction Valley Approach study. <i>Molecular Physics</i> , 2019, 117, 1172-1192. | 0.8 | 22 |
| 13306 | Quantum Chemistry Meets Deep Learning for Complex Carbohydrate and Glycopeptide Species I. <i>Zeitschrift Fur Physikalische Chemie</i> , 2019, 233, 527-550. | 1.4 | 4 |
| 13307 | Raman, infrared and NMR spectra, vibrational assignments and quantum mechanical calculations of centrosymmetric 3,6-Dichloro-1,2,4,5-tetrazine. <i>Journal of Molecular Structure</i> , 2019, 1178, 298-304. | 1.8 | 1 |
| 13308 | Shedding Light on the Basis Set Dependence of the Minnesota Functionals: Differences Between Plane Waves, Slater Functions, and Gaussians. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 557-571. | 2.3 | 6 |
| 13309 | Novel nonmetal catalyst of supported tetraphenylphosphonium bromide for acetylene hydrochlorination. <i>Catalysis Science and Technology</i> , 2019, 9, 188-198. | 2.1 | 14 |
| 13310 | QMC-SW: A simple workflow for quantum Monte Carlo calculations in chemistry. <i>SoftwareX</i> , 2019, 9, 7-14. | 1.2 | 6 |
| 13311 | Performance of DFT for C₆₀ Isomerization Energies: A Noticeable Exception to Jacobâ€™s Ladder. <i>Journal of Physical Chemistry A</i> , 2019, 123, 257-266. | 1.1 | 19 |
| 13312 | Direct Single- and Double-Side Triol-Functionalization of the Mixed Type Anderson Polyoxotungstate [Cr(OH)₃W₆O₂₁]^{6â€“}. <i>Inorganic Chemistry</i> , 2019, 58, 106-113. | 1.9 | 20 |
| 13313 | Revisited Mechanism of Reaction between a Model Lysine Amino Acid Side Chain and 4-Hydroxynonenal in Different Solvent Environments. <i>Journal of Organic Chemistry</i> , 2019, 84, 526-535. | 1.7 | 14 |
| 13314 | Thermally Activated Delayed Fluorescence (Green) in Undoped Film and Exciplex Emission (Blue) in Acridoneâ€™Carbazole Derivatives for OLEDs. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1003-1014. | 1.5 | 36 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 13315 | Valence $\pi\pi^*$ Excitations in Benzene Studied by Multiconfiguration Pair-Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 75-81. | 2.1 | 29 |
| 13316 | Angle-resolved photoelectron spectroscopy and scanning tunnelling spectroscopy studies of the endohedral fullerene Li@C ₆₀ . <i>Nanoscale</i> , 2019, 11, 2668-2678. | 2.8 | 16 |
| 13317 | Asymmetric Oxidation of Enol Derivatives to α -Alkoxy Carbonyls Using Iminium Salt Catalysts: A Synthetic and Computational Study. <i>Journal of Organic Chemistry</i> , 2019, 84, 544-559. | 1.7 | 8 |
| 13318 | Designing Reactions with Post-Transition-State Bifurcations: Asynchronous Nitrene Insertions into C π -C σ Bonds. <i>CheM</i> , 2019, 5, 227-236. | 5.8 | 28 |
| 13319 | Anharmonicity of the bonded O H group vibrations in water dimer. DFT study including dispersion interaction. <i>Journal of Molecular Liquids</i> , 2019, 277, 269-279. | 2.3 | 5 |
| 13320 | Hydrogen Activation by Silica-Supported Metal Ion Catalysts: Catalytic Properties of Metals and Performance of DFT Functionals. <i>Journal of Physical Chemistry A</i> , 2019, 123, 171-186. | 1.1 | 3 |
| 13321 | Highly efficient capturing and adsorption of cesium and strontium ions from aqueous solution by porous organic cage: A combined experimental and theoretical study. <i>Applied Surface Science</i> , 2019, 471, 726-732. | 3.1 | 15 |
| 13322 | Assessment of a set of twelve density functionals to estimate the global reactivity of myricetin through the Koopmans's theorem. <i>Chemical Physics Letters</i> , 2019, 715, 354-359. | 1.2 | 11 |
| 13323 | Quadrupolar ^{14}N NMR Relaxation from Force-Field and Ab Initio Molecular Dynamics in Different Solvents. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 509-519. | 2.3 | 17 |
| 13324 | Description of Potential Energy Surfaces of Molecules Using FFLUX Machine Learning Models. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 116-126. | 2.3 | 16 |
| 13325 | Electron-Spin Structure and Metal-Ligand Bonding in Open-Shell Systems from Relativistic EPR and NMR: A Case Study of Square-Planar Iridium Catalysts. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 201-214. | 2.3 | 17 |
| 13326 | 1,2-H Atom Rearrangements in Benzyloxyl Radicals. <i>Journal of Physical Chemistry A</i> , 2019, 123, 492-504. | 1.1 | 5 |
| 13327 | Generalized Hartree-Fock with Nonperturbative Treatment of Strong Magnetic Fields: Application to Molecular Spin Phase Transitions. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 348-356. | 2.3 | 33 |
| 13328 | Exfoliated Triazine-Based Covalent Organic Nanosheets with Multielectron Redox for High-Performance Lithium Organic Batteries. <i>Advanced Energy Materials</i> , 2019, 9, 1801010. | 10.2 | 174 |
| 13329 | Ouroboros: Heterocycles closed by dative σ bonds and stabilized by π delocalization. <i>Tetrahedron</i> , 2019, 75, 335-345. | 1.0 | 6 |
| 13330 | Investigations of Stacked DNA Base-Pair Steps: Highly Accurate Stacking Interaction Energies, Energy Decomposition, and Many-Body Stacking Effects. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 95-115. | 2.3 | 55 |
| 13331 | Generalized Gradient Approximation Exchange Energy Functional with Near-Best Semilocal Performance. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 303-310. | 2.3 | 24 |
| 13332 | Photoregeneration of Biomimetic Nicotinamide Adenine Dinucleotide Analogues via a Dye-Sensitized Approach. <i>ACS Applied Energy Materials</i> , 2019, 2, 80-91. | 2.5 | 15 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13333 | Interstellar dimethyl ether gas-phase formation: a quantum chemistry and kinetics study. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019, 482, 3567-3575. | 1.6 | 48 |
| 13334 | Bacterio- and Isobacteriodilactones by Stepwise or Direct Oxidations of <i>meso</i> -Tetrakis(pentafluorophenyl)porphyrin. <i>Journal of Organic Chemistry</i> , 2019, 84, 239-256. | 1.7 | 23 |
| 13335 | Performance of time-dependent density functional theory on twisted intramolecular charge transfer state of emerging visible light photoswitches. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 371, 336-340. | 2.0 | 9 |
| 13336 | A theoretical investigation on the thermally activated delayed fluorescence characteristics of the isomers of DTCBP _y . <i>Journal of Molecular Graphics and Modelling</i> , 2019, 86, 125-131. | 1.3 | 5 |
| 13337 | Identification of potential drugs targeting L-Lysine diaminopimelate aminotransferase of <i>Chlamydia trachomatis</i> : An integrative pharmacoinformatics approach. <i>Journal of Cellular Biochemistry</i> , 2019, 120, 2271-2288. | 1.2 | 14 |
| 13338 | TD-DFT: An iterative vector interaction method for exterior/interior roots of TD-DFT. <i>Journal of Computational Chemistry</i> , 2019, 40, 1023-1037. | 1.5 | 18 |
| 13339 | The reHISS Three-Range Exchange Functional with an Optimal Variation of Hartree-Fock and Its Use in the reHISS Density Functional Theory Method. <i>Journal of Computational Chemistry</i> , 2019, 40, 29-38. | 1.5 | 7 |
| 13340 | Azobased iminopyridine ligands and their rhenium metal complexes: Syntheses, spectroscopic, trans-cis photoisomerization and theoretical studies. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 368, 78-84. | 2.0 | 8 |
| 13341 | Maximal orbital analysis of molecular wavefunctions. <i>Journal of Computational Chemistry</i> , 2019, 40, 39-50. | 1.5 | 3 |
| 13342 | Role of sterics in phosphine-ligated gold clusters. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 1689-1699. | 1.3 | 17 |
| 13343 | Design and Synthesis of Coumarin-Imidazole Hybrid Chromophores: Solvatochromism, Acidochromism and Nonlinear Optical Properties. <i>Photochemistry and Photobiology</i> , 2019, 95, 740-754. | 1.3 | 17 |
| 13344 | Derivatization reagent-assisted enantioseparation of 3-hydroxyaspartate with two chiral centers in rat cerebrospinal fluid by capillary electrophoresis-mass spectrometry. <i>Analytica Chimica Acta</i> , 2019, 1047, 257-266. | 2.6 | 18 |
| 13345 | Identification of selective MMP-9 inhibitors through multiple e-pharmacophore, ligand-based pharmacophore, molecular docking, and density functional theory approaches. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 944-965. | 2.0 | 34 |
| 13346 | Pivotal role of intramolecular catalysis in the selective acetylation of alkyl amines. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3842. | 0.9 | 0 |
| 13347 | Prebiotic chemistry and origins of life research with atomistic computer simulations. <i>Physics of Life Reviews</i> , 2020, 34-35, 105-135. | 1.5 | 25 |
| 13348 | The static parallel distribution algorithms for hybrid density-functional calculations in HONPAS package. <i>International Journal of High Performance Computing Applications</i> , 2020, 34, 159-168. | 2.4 | 2 |
| 13349 | Vibrational coherence and quantum yield of retinal-chromophore-inspired molecular switches. <i>Faraday Discussions</i> , 2019, 221, 299-321. | 1.6 | 12 |
| 13350 | A Systematic Study of Electronic Structure for Anti-cancer Drug Molecule 5-Fluorouracil Within Various Solvents from First-Principles Calculations. <i>IFMBE Proceedings</i> , 2020, , 721-726. | 0.2 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13351 | Structural, Vibrational and UV/Vis Studies of Adamantane-Containing Triazole Thiones by Spectral, DFT and Multi-reference <i>ab initio</i> Methods. <i>Zeitschrift Fur Physikalische Chemie</i> , 2020, 234, 85-106. | 1.4 | 2 |
| 13352 | Simulation of Vacuum Ultraviolet Absorption Spectra: Paraffin, Isoparaffin, Olefin, Naphthene, and Aromatic Hydrocarbon Class Compounds. <i>Applied Spectroscopy</i> , 2020, 74, 72-80. | 1.2 | 12 |
| 13353 | SLMP53-1 interacts with wild-type and mutant p53 DNA-binding domain and reactivates multiple hotspot mutations. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2020, 1864, 129440. | 1.1 | 13 |
| 13354 | Polydopamine-induced growth of mineralized Fe^{3+} -FeOOH nanorods for construction of silk fabric with excellent superhydrophobicity, flame retardancy and UV resistance. <i>Chemical Engineering Journal</i> , 2020, 382, 122988. | 6.6 | 65 |
| 13355 | Gas phase detection of chemical warfare agents CWAs with portable Raman. <i>Journal of Hazardous Materials</i> , 2020, 384, 121279. | 6.5 | 33 |
| 13356 | Amphiphilic hyper-crosslinked porous cyclodextrin polymer with high specific surface area for rapid removal of organic micropollutants. <i>Chemical Engineering Journal</i> , 2020, 382, 123015. | 6.6 | 62 |
| 13357 | Structural characterisation and theoretical study of a dinuclear copper(II) complex bridged by meta-phenylenediiminophenolate moiety. <i>Journal of Molecular Structure</i> , 2020, 1199, 126996. | 1.8 | 7 |
| 13358 | First-principles approach to the first step of metal-phosphine bond formation to synthesize alloyed quantum dots using dissimilar metal precursors. <i>Chemical Physics</i> , 2020, 528, 110512. | 0.9 | 0 |
| 13359 | Design, theoretical study and correlation of the electronic and optical properties of diethynylphenylthiophene as photovoltaic materials. <i>Journal of Molecular Structure</i> , 2020, 1201, 127093. | 1.8 | 3 |
| 13360 | Interaction of aromatic compounds and anions with naphthylimide-dansylamide fluorescent dyad: Experimental evidence of aryl π - π^* and aryl π -anion contacts and DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 226, 117553. | 2.0 | 0 |
| 13361 | Scalable synthesis of multi-substituted aryl-phosphonates: Exploring the limits of isoretical expansion and the synthesis of new triazene-based phosphonates. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2020, 195, 231-244. | 0.8 | 1 |
| 13362 | Aufbau Principle for Diffuse Electrons of Double-Shell Metal Ammonia Complexes: The Case of $M(\text{NH}_3)_4 @ 12\text{NH}_3$, $M = \text{Li}, \text{Be}^{2+}$. <i>Journal of Physical Chemistry A</i> , 2020, 124, 505-512. | 1.1 | 23 |
| 13363 | Synthesis, Photophysical and Electronic Properties of New Red-NIR Emitting Donor-Acceptor Pyrene Derivatives. <i>Chemistry - A European Journal</i> , 2020, 26, 438-453. | 1.7 | 33 |
| 13364 | The Chronus Quantum software package. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1436. | 6.2 | 66 |
| 13365 | Mechanism of sulfonation-induced chain scission of selectively oxidized polysaccharides. <i>Carbohydrate Polymers</i> , 2020, 229, 115503. | 5.1 | 11 |
| 13366 | Mechanistic insights into the origin of substituent-directed product E selectivity for gold-catalyzed [4+1]-annulations of 1,4-diyne-3-ols with isoxazoles: A DFT study. <i>Molecular Catalysis</i> , 2020, 480, 110647. | 1.0 | 5 |
| 13367 | A combination of FTIR and DFT to study the microscopic structure and hydrogen-bonding interaction properties of the [BMIM][BF ₄] and water. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 226, 117624. | 2.0 | 21 |
| 13368 | Gas-phase structures and thermochemical properties of protonated 5-HMF isomers. <i>International Journal of Mass Spectrometry</i> , 2020, 447, 116237. | 0.7 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13369 | The structure and interaction properties of two task-specific ionic liquids and acetonitrile mixtures: A combined FTIR and DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 226, 117641. | 2.0 | 25 |
| 13370 | Ultrafast nonadiabatic dynamics probed by nitrogen K-edge absorption spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 2667-2676. | 1.3 | 34 |
| 13371 | Intra- and Intermolecular Fluorescence Quenching of Alkylthio-Substituted Phthalimides by Photoinduced Electron Transfer: Distance, Position and Conformational Dependence. <i>ChemPhotoChem</i> , 2020, 4, 89-97. | 1.5 | 2 |
| 13372 | A computational study of gas-phase acidity and basicity of azulene-based uracil analogue. <i>Structural Chemistry</i> , 2020, 31, 319-328. | 1.0 | 3 |
| 13373 | Thioether-linked liquid crystal dimers and trimers: The twist-bend nematic phase. <i>Journal of Molecular Structure</i> , 2020, 1199, 126913. | 1.8 | 42 |
| 13374 | Making machine learning a useful tool in the accelerated discovery of transition metal complexes. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1439. | 6.2 | 34 |
| 13375 | Tunable fluorescent pyrene/diarylethene-based bistable [3]rotaxane. <i>Dyes and Pigments</i> , 2020, 172, 107800. | 2.0 | 12 |
| 13376 | Temperature dependence of the vibrational spectrum of porphycene: a qualitative failure of classical-nuclei molecular dynamics. <i>Faraday Discussions</i> , 2020, 221, 526-546. | 1.6 | 22 |
| 13377 | Contributions of Computer-Based Chemical Modeling Technologies on the Risk Assessment and the Environmental Fate Study of (Nano)pesticides. , 2020, , 1-27. | | 3 |
| 13378 | Enumeration of <i>de novo</i> inorganic complexes for chemical discovery and machine learning. <i>Molecular Systems Design and Engineering</i> , 2020, 5, 139-152. | 1.7 | 23 |
| 13379 | Copper(II) complexes containing pyridine-based and phenolate-based systems: Synthesis, characterization, DFT study, biomimetic catalytic activity of catechol oxidase and phenoxazinone synthase. <i>Journal of the Chinese Chemical Society</i> , 2020, 67, 135-151. | 0.8 | 7 |
| 13380 | A study on hydrogen uptake and release of a eutectic mixture of biphenyl and diphenyl ether. <i>Journal of Energy Chemistry</i> , 2020, 42, 11-16. | 7.1 | 20 |
| 13381 | An experimental and computational study of the effect of aqueous solution on the multiphoton ionisation photoelectron spectrum of phenol. <i>Faraday Discussions</i> , 2019, 221, 202-218. | 1.6 | 7 |
| 13382 | Computational simulation of mechanism and isotope effects on acetal heterolysis as a model for glycoside hydrolysis. <i>Pure and Applied Chemistry</i> , 2020, 92, 75-84. | 0.9 | 2 |
| 13383 | Regioselective cyclization reaction of 2-imino-2H-chromene-3-carboxamide with triethyl phosphonoacetate; a combined spectral and computational studies. <i>Journal of Molecular Structure</i> , 2020, 1199, 126935. | 1.8 | 1 |
| 13384 | Quantum chemical calculation studies of Pd _n Si ₁₂ (n = 1-3) clusters: effects of doping Pd atoms on the structural and electronic properties. <i>Molecular Physics</i> , 2020, 118, e1656350. | 0.8 | 2 |
| 13385 | Structural, spectroscopic and theoretical studies of sodium (2-carbamoylphenoxy) acetate salt. <i>Journal of Molecular Structure</i> , 2020, 1200, 127016. | 1.8 | 1 |
| 13386 | Diverse coordination of aroylhydrazones toward iron(III) in solid state and in solution: spectrometric, spectroscopic and computational study. <i>Molecular Diversity</i> , 2020, 24, 1253-1263. | 2.1 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13387 | Investigation of midazolam electro-oxidation on boron doped diamond electrode by voltammetric techniques and density functional theory calculations: Application in beverage samples. <i>Talanta</i> , 2020, 207, 120319. | 2.9 | 10 |
| 13388 | Density Functional Studies of Coenzyme NADPH and Its Oxidized Form NADP ⁺ : Structures, UV-Vis Spectra, and the Oxidation Mechanism of NADPH. <i>Journal of Computational Chemistry</i> , 2020, 41, 305-316. | 1.5 | 13 |
| 13389 | Relationships between Anhydrous and Solvated Species of Dexketoprofen Trometamol: A Solid-State Point of View. <i>Crystal Growth and Design</i> , 2020, 20, 226-236. | 1.4 | 11 |
| 13390 | A combined experimental and DFT computations study of novel (E)-3-(benzofuran-2-yl)-2-(thiophen-2-yl)acrylonitrile (TACNBNF): Insight into the synthesis, single crystal XRD, NMR, vibrational spectral analysis, in vitro antioxidant and in silico molecular docking investigation with human peroxiredoxin 5 protein. <i>Journal of Molecular Structure</i> , 2020, 1202, 127241. | 1.8 | 16 |
| 13391 | Enantioselective Synthesis of Complex Fused Heterocycles through Chiral Phosphoric Acid Catalyzed Intramolecular Inverse Electron Demand Aza-Diels-Alder Reactions. <i>Chemistry - A European Journal</i> , 2020, 26, 1406-1413. | 1.7 | 15 |
| 13392 | Mechanism and Stereoselectivity of the Elementometalation Process of Activated Alkyne $R_1C\equiv\frac{1}{2}CR(R_2\frac{3}{4}CO_2)Tj$. <i>ETQq110784314</i> | 1.5 | 7 |
| 13393 | Construction of a metallic silver nanoparticle-decorated bismuth oxybromide-based composite material as a readily recyclable photocatalyst. <i>Journal of Cleaner Production</i> , 2020, 246, 119007. | 4.6 | 24 |
| 13394 | Prediction of octanol-air partition coefficients for PCBs at different ambient temperatures based on the solvation free energy and the dimer ratio. <i>Chemosphere</i> , 2020, 242, 125246. | 4.2 | 6 |
| 13395 | The effect of the change in substituents' positions on the formation of supramolecular networks and the solvent type/substituent dependence of prototropic behavior in three new o-hydroxy Schiff bases. <i>Journal of Molecular Structure</i> , 2020, 1200, 127109. | 1.8 | 7 |
| 13396 | A comprehensive mechanism for liquid-phase decomposition of 1,3,5,7-tetranitro-1,3,5,7-tetraoctane (HMX): Thermolysis experiments and detailed kinetic modeling. <i>Combustion and Flame</i> , 2020, 212, 67-78. | 2.8 | 16 |
| 13397 | Three-dimensional hydrogen-bonded magnesium(II) supramolecular motifs based on in situ generated alkanesulfonate (Me/Et/ PrSO ₃ ⁻) ligands: A combined experimental and computational study. <i>Polyhedron</i> , 2020, 175, 114200. | 1.0 | 1 |
| 13398 | QCMS ² as a new method for providing insight into peptide fragmentation: The influence of the side-chain and inter-side-chain interactions. <i>Journal of Mass Spectrometry</i> , 2020, 55, e4446. | 0.7 | 4 |
| 13399 | In situ visualization and real-time tracking of emulsion and miniemulsion polymerization at the microscale via fluorescence imaging. <i>Chemical Engineering Science</i> , 2020, 211, 115288. | 1.9 | 8 |
| 13400 | From a week to less than a day: Speedup and scaling of coordinate-scaled exact exchange calculations in plane waves. <i>Computer Physics Communications</i> , 2020, 247, 106943. | 3.0 | 5 |
| 13401 | Dynamical fluxionality, multiplicity of geometrical forms, and electronic properties of anionic, neutral, and cationic Ta _n Si ₁₂ (n = 1-3) clusters: quantum chemical calculations. <i>Molecular Physics</i> , 2020, 118, e1682209. | 0.8 | 6 |
| 13402 | Spin-crossover behavior of bis[dihydrobis(4-methylpyrazol-1-yl-borate)]-(2,2'-bipyridine)iron and analogous complexes in the bulk and in thin films: Elucidating the influence of π - π -interactions on the type of spin transition. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 094001. | 0.7 | 4 |
| 13403 | Estimating Systematic Error and Uncertainty in <i>Ab Initio</i> Thermochemistry: II. ATOMIC(hc) Enthalpies of Formation for a Large Set of Hydrocarbons. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 399-426. | 2.3 | 28 |
| 13404 | Implementation of the Coupled-Cluster Method with Single, Double, and Triple Excitations using Tensor Decompositions. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 453-467. | 2.3 | 23 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13405 | Elucidation of the Mechanism of Silver-Catalyzed Inverse Electron-Demand Diels-Alder (IEDDA) Reaction of 1,2-Diazines and Siloxy Alkynes. <i>ChemCatChem</i> , 2020, 12, 366-372. | 1.8 | 3 |
| 13406 | Cyclometalated Iridium Bipyridine Complexes with Peripheral Antimony Substituents. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2020, 646, 636-641. | 0.6 | 3 |
| 13407 | The mechanism of water loss from protonated cationones. <i>Rapid Communications in Mass Spectrometry</i> , 2020, 34, e8617. | 0.7 | 4 |
| 13408 | Nickel-mediated cross-coupling via C=O activation assisted by organoaluminum. <i>Journal of the Chinese Chemical Society</i> , 2020, 67, 376-382. | 0.8 | 3 |
| 13409 | Poly(1,3,5-tris(4-ethynylphenyl)-benzene) Conjugated Polymers as Electrochemical Sensors for Hydrogen Peroxide Detection. <i>ACS Applied Polymer Materials</i> , 2020, 2, 685-690. | 2.0 | 7 |
| 13410 | Ab Initio Analysis of Metal-Ligand Bonding in An(COT) ₂ with An=Th, U in Their Ground and Core-Excited States. <i>Chemistry - A European Journal</i> , 2020, 26, 1776-1788. | 1.7 | 23 |
| 13411 | Influence of Electrolyte Composition on Ultrafast Interfacial Electron Transfer in Fe-Sensitized TiO ₂ -Based Solar Cells. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1794-1811. | 1.5 | 19 |
| 13412 | One-bond ¹ J(¹⁵ N) spin-spin coupling constants of cationic fluorinating reagents: Insights from DFT calculations. <i>Magnetic Resonance in Chemistry</i> , 2020, 58, 548-558. | 1.1 | 3 |
| 13413 | Interconnection of the Antenna Pigment 8-HDF and Flavin Facilitates Red-Light Reception in a Bifunctional Animal-like Cryptochrome. <i>Biochemistry</i> , 2020, 59, 594-604. | 1.2 | 10 |
| 13414 | Cu ₄ I ₄ -cubane clusters based on 10-(aryl)phenoxarsines and their luminescence. <i>Dalton Transactions</i> , 2020, 49, 482-491. | 1.6 | 21 |
| 13415 | A simple D-A system of phenanthroimidazole- <i>h</i> -fluorenone for highly efficient non-doped bipolar AIE luminogens: synthesis, and molecular optical, thermal and electrochemical properties. <i>New Journal of Chemistry</i> , 2020, 44, 1785-1794. | 1.4 | 11 |
| 13416 | Mechanism and stereoselectivity of benzylic C-H hydroxylation by Ru-porphyrin: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 346-352. | 1.5 | 8 |
| 13417 | Synthesis, characterization and C-H amination reactivity of nickel iminyl complexes. <i>Chemical Science</i> , 2020, 11, 1260-1268. | 3.7 | 43 |
| 13418 | Reactions of a distonic peroxy radical anion influenced by SOMO-HOMO conversion: an example of anion-directed channel switching. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 2130-2141. | 1.3 | 9 |
| 13419 | Solvent-free hydrogenation of levulinic acid to β -valerolactone using a Shvo catalyst precursor: optimization, thermodynamic insights, and life cycle assessment. <i>Green Chemistry</i> , 2020, 22, 2443-2458. | 4.6 | 22 |
| 13420 | Dinuclear copper(II) complex with a benzimidazole derivative: Crystal structure, theoretical calculations, and cytotoxic activity. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5425. | 1.7 | 7 |
| 13421 | The Bursten model of ligand additivity applied to orbital energetics of octahedral d6 phosphine complexes. <i>Inorganica Chimica Acta</i> , 2020, 502, 119349. | 1.2 | 1 |
| 13422 | Metal ion substitution and aldehyde exchange for CuII ₄ aggregates from two types of piperazine-based Schiff base ligands: Synthesis, X-ray structures, magnetic studies and theoretical validation. <i>Inorganica Chimica Acta</i> , 2020, 503, 119439. | 1.2 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13423 | Solubility and solvation free energy of a cardiovascular drug, LASSBio-294, in ionic liquids: A computational study. <i>Journal of Molecular Liquids</i> , 2020, 301, 112449. | 2.3 | 32 |
| 13424 | A new phenothiazine-based selective visual and fluorescent sensor for cyanide. <i>BMC Chemistry</i> , 2020, 14, 2. | 1.6 | 16 |
| 13425 | Substitution Effects on the Optoelectronic Properties of Coumarin Derivatives. <i>Applied Sciences (Switzerland)</i> , 2020, 10, 144. | 1.3 | 17 |
| 13426 | Accelerated C ₂ H ₂ /CO ₂ Separation by a Se-Functionalized Porous Coordination Polymer with Low Binding Energy. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 3764-3772. | 4.0 | 58 |
| 13427 | Structural and reorientational dynamics of tetrahydroborate (BH ₄ ⁻) and tetrahydrofuran (THF) in a Mg(BH ₄) ₂ ·3THF adduct: neutron-scattering characterization. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 368-378. | 1.3 | 6 |
| 13428 | Molecular simulations of analyte partitioning and diffusion in liquid crystal sensors. <i>Molecular Systems Design and Engineering</i> , 2020, 5, 304-316. | 1.7 | 14 |
| 13429 | Structural, electrochemical and photophysical behavior of Ru(II) complexes with large bite angle sulfur-bridged terpyridyl ligands. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 117-127. | 3.0 | 6 |
| 13430 | Light-induced disruption of an acyl hydrazone link as a novel strategy for drug release and activation: isoniazid as a proof-of-concept case. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 859-870. | 3.0 | 12 |
| 13431 | A Ni/Fe-based heterometallic phthalocyanine conjugated polymer for the oxygen evolution reaction. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 642-646. | 3.0 | 32 |
| 13432 | Diversity-oriented approach to functional thiophene dyes by Suzuki coupling-lithiation one-pot sequences. <i>Organic Chemistry Frontiers</i> , 2020, 7, 329-339. | 2.3 | 8 |
| 13433 | An excited state managing molecular design platform of blue thermally activated delayed fluorescence emitters by I-linker engineering. <i>Journal of Materials Chemistry C</i> , 2020, 8, 1736-1745. | 2.7 | 14 |
| 13434 | Thiazolidine-4-one clubbed pyrazoles hybrids: Potent α -amylase and α -glucosidase inhibitors with NLO properties. <i>Journal of Heterocyclic Chemistry</i> , 2020, 57, 1573-1587. | 1.4 | 31 |
| 13435 | Effect of 1-ethyl-3-methylimidazolium acetate on the oxidation of caffeic acid benzyl ester: An electrochemical and theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4044. | 0.9 | 3 |
| 13436 | Benchmark study of DFT and composite methods for bond dissociation energies in argon compounds. <i>Chemical Physics</i> , 2020, 531, 110676. | 0.9 | 8 |
| 13437 | A DFT investigation on magnetoelectric coupling in PbBO ₃ (B ^A = ^A V, Cr, Mn, Co, and Cu) materials: The influence on multiferroic properties. <i>Journal of Magnetism and Magnetic Materials</i> , 2020, 500, 166364. | 1.0 | 9 |
| 13438 | Determinants of the Lead(II) Affinity in <i>pbrR</i> Protein: A Computational Study. <i>Inorganic Chemistry</i> , 2020, 59, 790-800. | 1.9 | 19 |
| 13439 | Molecule to Supramolecule: Chirality Induction, Inversion, and Amplification in a Mg(II)porphyrin Dimer Templated by Chiral Diols. <i>Inorganic Chemistry</i> , 2020, 59, 801-809. | 1.9 | 13 |
| 13440 | Performance of the LRESC Model on top of DFT Functionals for Relativistic NMR Shielding Calculations. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 722-730. | 2.5 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13441 | Isopimarane Diterpenoids from the Rhizomes of <i>Kaempferia marginata</i> and Their Potential Anti-inflammatory Activities. <i>Journal of Natural Products</i> , 2020, 83, 14-19. | 1.5 | 19 |
| 13442 | Mechanism of Cobalt-Catalyzed Direct Aminocarbonylation of Unactivated Alkyl Electrophiles: Outer-Sphere Amine Substitution To Form Amide Bond. <i>ACS Catalysis</i> , 2020, 10, 1520-1527. | 5.5 | 18 |
| 13443 | Polaron and Exciton Delocalization in Oligomers of High-Performance Polymer PTB7. <i>Journal of the American Chemical Society</i> , 2020, 142, 1359-1366. | 6.6 | 5 |
| 13444 | Towards a Stronger Halogen Bond Involving Astatine: Unexpected Adduct with Bu ₃ PO Stabilized by Hydrogen Bonding. <i>Chemistry - A European Journal</i> , 2020, 26, 3713-3717. | 1.7 | 13 |
| 13445 | Effect of the Solute Cavity on the Solvation Energy and its Derivatives within the Framework of the Gaussian Charge Scheme. <i>Journal of Computational Chemistry</i> , 2020, 41, 922-939. | 1.5 | 86 |
| 13446 | Experimental Evidence for the Incorporation of Two Metals at Equivalent Lattice Positions in Mixed-Metal Organic Frameworks. <i>Chemistry - A European Journal</i> , 2020, 26, 5667-5675. | 1.7 | 9 |
| 13447 | Spirocyclic lactams and curvulinic acid derivatives from the endophytic fungus <i>Curvularia lunata</i> and their antibacterial and antifungal activities. <i>Fä-toterapÄ-Äç</i> , 2020, 141, 104466. | 1.1 | 7 |
| 13448 | Amine derivative of triphenyl ether as an optical sensor for the detection of cyanide ions and traces of water in acetonitrile supported with voltammetric studies. <i>Journal of Applied Electrochemistry</i> , 2020, 50, 185-195. | 1.5 | 9 |
| 13449 | Cost-Effective Potential for Accurate Polarizable Embedding Calculations in Protein Environments. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1162-1174. | 2.3 | 12 |
| 13450 | Novel ferrocene-based 1,2,3-triazolyl compounds: Synthesis, anti-migration properties and catalytic effects on oxidizers during combustion. <i>Inorganica Chimica Acta</i> , 2020, 502, 119374. | 1.2 | 18 |
| 13451 | Unveiling the Relationship between Energy Transfer and the Triplet Energy Level by Tuning Diarylethene within Europium(III) Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 661-668. | 1.9 | 9 |
| 13452 | The physical structure and surface reactivity of graphene oxide. <i>Diamond and Related Materials</i> , 2020, 101, 107613. | 1.8 | 7 |
| 13453 | Application of vacuum-ultraviolet (VUV) for phenolic homologues removal in humic acid solution: Efficiency, pathway and DFT calculation. <i>Journal of Hazardous Materials</i> , 2020, 384, 121464. | 6.5 | 17 |
| 13454 | <i>Ab initio</i> calculation of electrostatic potentials for C ₆₀ and C ₈₀ . <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2020, 53, 035102. | 0.6 | 10 |
| 13455 | Thermal decomposition characteristics and kinetic analysis of C ₄ F ₇ N/CO ₂ gas mixture. <i>Journal Physics D: Applied Physics</i> , 2020, 53, 055502. | 1.3 | 19 |
| 13456 | Visualizing biomolecular electrostatics in virtual reality with UnityMolâ€APBS. <i>Protein Science</i> , 2020, 29, 237-246. | 3.1 | 31 |
| 13457 | Rational design, synthesis and biological profiling of new KDM4C inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2020, 28, 115128. | 1.4 | 9 |
| 13458 | Spectral and computational studies on regioselective synthesis of 4-oxo-6-phenyl-2-selenoxo-1,2,3,4-tetrahydropyrimidine-5-carbonitrile. <i>Journal of Molecular Structure</i> , 2020, 1203, 127408. | 1.8 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13459 | Hydrogen bond analysis of a third order nonlinear optical crystal, 2-amino-5-bromopyridinium benzilate, using structural and computational characterizations. <i>Journal of Molecular Structure</i> , 2020, 1203, 127419. | 1.8 | 4 |
| 13460 | Silicon carbide nanobelt: A novel molecule with potential technological application. <i>Computational and Theoretical Chemistry</i> , 2020, 1171, 112645. | 1.1 | 4 |
| 13461 | A Minimal Membrane Metal Transport System: Dynamics and Energetics of <i>mer</i> Proteins. <i>Journal of Computational Chemistry</i> , 2020, 41, 528-537. | 1.5 | 5 |
| 13462 | Dinuclear ruthenium(II) polypyridyl complexes: Mechanistic study with biomolecules, DNA/BSA interactions and cytotoxic activity. <i>Polyhedron</i> , 2020, 178, 114334. | 1.0 | 18 |
| 13463 | Self-assembly of amphiphilic aryl-squaramides in water driven by dipolar π - π interactions. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 888-894. | 1.5 | 16 |
| 13464 | Statistical molecular fragmentation: which parameters influence the branching ratios?. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 3160-3172. | 1.3 | 7 |
| 13465 | Thermal, electronic and thermoelectric properties of TiNiSn and TiCoSb based quaternary half Heusler alloys obtained from <i>ab initio</i> calculations. <i>Sustainable Energy and Fuels</i> , 2020, 4, 895-910. | 2.5 | 15 |
| 13466 | A Novel, Modified Human Butyrylcholinesterase Catalytically Degrades the Chemical Warfare Nerve Agent, Sarin. <i>Toxicological Sciences</i> , 2020, 174, 133-146. | 1.4 | 5 |
| 13467 | Understanding Beam-Induced Electronic Excitations in Materials. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1200-1214. | 2.3 | 13 |
| 13468 | Exploring the Reactivity and Biological Effects of Heteroleptic π -Heterocyclic Carbene Gold(I)-Alkynyl Complexes. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 1040-1051. | 1.0 | 26 |
| 13469 | Photolysis of 3-(1-cyclohexyl-5-aryloxy-3-pyrazolinyl)coumarins: Effective Fluorescence Decay. <i>Photochemistry and Photobiology</i> , 2020, 96, 798-804. | 1.3 | 2 |
| 13470 | Computational Investigations of the Chemical Mechanism of the Enzyme Nitrogenase. <i>ChemBioChem</i> , 2020, 21, 1671-1709. | 1.3 | 36 |
| 13471 | Phosphorescent heteroleptic iridium(III) cyclometallates: Improved syntheses of acetylacetonate complexes and quantum chemical studies of their excited state properties. <i>Polyhedron</i> , 2020, 176, 114256. | 1.0 | 4 |
| 13472 | Formyltetrahydrofolate Decarboxylase Synthesizes the Active Site CO Ligand of O_2 -Tolerant [NiFe] Hydrogenase. <i>Journal of the American Chemical Society</i> , 2020, 142, 1457-1464. | 6.6 | 24 |
| 13473 | Hypervalent halogen hydrides HalHn (Hal = Cl, Br, I; n = 3, 5, 7): DFT and <i>ab initio</i> stability prediction. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1. | 0.5 | 2 |
| 13474 | Discovering Biomolecules with <i>Huisgenase</i> Activity: Designed Repeat Proteins as Biocatalysts for (3 + 2) Cycloadditions. <i>Journal of the American Chemical Society</i> , 2020, 142, 762-776. | 6.6 | 8 |
| 13475 | Empirical Double-Hybrid Density Functional Theory: A "Third Way" in Between WFT and DFT. <i>Israel Journal of Chemistry</i> , 2020, 60, 787-804. | 1.0 | 129 |
| 13476 | DFT/TDDFT investigation on the "A" type molecule probes 4-(5-R-thiophen-2-yl)-2-isobutyl-2H-[1,2,3]triazolo[4,5-e][1,2,4] triazolo[1,5-a]pyrimidines: fluorescence sensing mechanism and roles of weak interactions. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1. | 0.5 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13477 | New theoretical insights on tautomerism of hyperforin—a prenylated phloroglucinol derivative which may be responsible for St. John's wort (Hypericum perforatum) antidepressant activity. Structural Chemistry, 2020, 31, 657-666. | 1.0 | 6 |
| 13478 | Rapid removal of toxic metals Cu ²⁺ and Pb ²⁺ by amino trimethylene phosphonic acid intercalated layered double hydroxide: A combined experimental and DFT study. Chemical Engineering Journal, 2020, 392, 123711. | 6.6 | 147 |
| 13479 | Crystal structures and DFT analysis of Palladium(II) complexes with Schiff bases derived from N,N-dialkyl-p-phenylenediamines. Journal of Molecular Structure, 2020, 1204, 127549. | 1.8 | 15 |
| 13480 | Benchmarking Electronic Structure Methods for Accurate Fixed-Charge Electrostatic Models. Journal of Chemical Information and Modeling, 2020, 60, 249-258. | 2.5 | 12 |
| 13481 | A Topological Data Analysis perspective on noncovalent interactions in relativistic calculations. International Journal of Quantum Chemistry, 2020, 120, e26133. | 1.0 | 16 |
| 13482 | Computational study of [(phenanthroline) ₂ Fe(III)(terephthalate)] ³⁺ binuclear complex. Structural Chemistry, 2020, 31, 809-821. | 1.0 | 1 |
| 13483 | Microsolvation, hydrogen bond dynamics and excited state hydrogen atom transfer mechanism of 2,4-dihydroxychalcone. Chemical Physics Letters, 2020, 739, 137030. | 1.2 | 3 |
| 13484 | Density functional approximations for consistent spin and oxidation states of oxoiron complexes. International Journal of Quantum Chemistry, 2020, 120, e26121. | 1.0 | 10 |
| 13485 | How accurate is density functional theory in predicting spin density? An insight from the prediction of hyperfine coupling constants. Journal of Molecular Modeling, 2020, 26, 10. | 0.8 | 18 |
| 13486 | Influencing the Self-Sorting Behavior of [2.2]Paracyclophane-Based Ligands by Introducing Isostructural Binding Motifs. Chemistry - A European Journal, 2020, 26, 3335-3347. | 1.7 | 12 |
| 13487 | Probing the Effect of Counterions on the Oxidation of Alcohols Using Oxoammonium Salts. European Journal of Organic Chemistry, 2020, 2020, 108-112. | 1.2 | 14 |
| 13488 | Theoretical study on cyclophane amide molecular receptors and its complexation behavior with TCNQ. Journal of Photochemistry and Photobiology B: Biology, 2020, 203, 111735. | 1.7 | 11 |
| 13489 | Accuracy of density functional theory methods for the calculation of magnetic exchange couplings in binuclear iron(III) complexes. Polyhedron, 2020, 176, 114194. | 1.0 | 18 |
| 13490 | Co-effects of the electron transfer and intersystem crossing on the photophysics of a phenothiazine based Hg ²⁺ sensor. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 229, 117939. | 2.0 | 4 |
| 13491 | Ab-initio studies of thermal unimolecular decomposition of furan: A complementary deterministic and stochastic master equation model. Fuel, 2020, 264, 116492. | 3.4 | 14 |
| 13492 | Self-Consistent Range-Separated Density-Functional Theory with Second-Order Perturbative Correction via the Optimized-Effective-Potential Method. Journal of Chemical Theory and Computation, 2020, 16, 211-223. | 2.3 | 15 |
| 13493 | Substituent Effect on Conformational Preferences in Ground and Excited States of Selected Schiff Bases: An Insight from Theoretical Calculations. Journal of Physical Chemistry A, 2020, 124, 63-73. | 1.1 | 6 |
| 13494 | Effect of Chemical Variations in the Structure of Poly(ethylene oxide)-Based Polymers on Lithium Transport in Concentrated Electrolytes. Chemistry of Materials, 2020, 32, 121-126. | 3.2 | 27 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 13495 | Methionine-montmorillonite composite – A novel material for efficient adsorption of lead ions. <i>Advanced Powder Technology</i> , 2020, 31, 708-717. | 2.0 | 27 |
| 13496 | Applications of Infrared Multiple Photon Dissociation (IRMPD) to the Detection of Posttranslational Modifications. <i>Chemical Reviews</i> , 2020, 120, 3261-3295. | 23.0 | 51 |
| 13497 | A FFLUX Water Model: Flexible, Polarizable and with a Multipolar Description of Electrostatics. <i>Journal of Computational Chemistry</i> , 2020, 41, 619-628. | 1.5 | 23 |
| 13498 | 7-Azaindole-3-carboxylic acid and its Pt(II) and Pd(II) complexes: Crystal structure of the ligand, vibrational spectra, DFT calculations and <i>in vitro</i> antiproliferative activity. <i>Journal of Molecular Structure</i> , 2020, 1203, 127441. | 1.8 | 3 |
| 13499 | Spectroscopic, structural, electronic and bioactive characteristics of 3,5-bis(2,5-dimethylphenyl)pyridine (1): An experimental and theoretical investigations. <i>Journal of Molecular Structure</i> , 2020, 1203, 127448. | 1.8 | 1 |
| 13500 | Kinetics and Thermodynamics of Reactions Involving Criegee Intermediates: An Assessment of Density Functional Theory and Ab Initio Methods Through Comparison with CCSDT(Q)/CBS Data. <i>Journal of Computational Chemistry</i> , 2020, 41, 328-339. | 1.5 | 13 |
| 13501 | Insights into high pressure gas adsorption properties of ZIF-67: Experimental and theoretical studies. <i>Microporous and Mesoporous Materials</i> , 2020, 294, 109867. | 2.2 | 40 |
| 13502 | Fluorine-incorporated interface enhances cycling stability of lithium metal batteries with Ni-rich NCM cathodes. <i>Nano Energy</i> , 2020, 67, 104309. | 8.2 | 101 |
| 13503 | A novel approach for the selective extraction of Li ⁺ from the leaching solution of spent lithium-ion batteries using benzo-15-crown-5 ether as extractant. <i>Separation and Purification Technology</i> , 2020, 237, 116325. | 3.9 | 54 |
| 13504 | Absolutely Localized Projection-Based Embedding for Excited States. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 385-398. | 2.3 | 43 |
| 13505 | Modelling of Ca ²⁺ -promoted structural effects in wild type and post-translationally modified Connexin26. <i>Molecular Simulation</i> , 2020, 46, 235-245. | 0.9 | 0 |
| 13506 | A Quadrupolar Bis-Triarylborane Chromophore as a Fluorimetric and Chiroptic Probe for Simultaneous and Selective Sensing of DNA, RNA and Proteins. <i>Chemistry - A European Journal</i> , 2020, 26, 2195-2203. | 1.7 | 33 |
| 13507 | Designing new donor materials based on functionalized DCCnT with different electron-donating groups: A density functional theory (DFT) and time dependent density functional theory (TDDFT)-based study. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26112. | 1.0 | 5 |
| 13508 | Synthesis of thioxopropanamide surfactants for studying the flotation performance and adsorption mechanism on chalcopyrite. <i>Applied Surface Science</i> , 2020, 505, 144539. | 3.1 | 23 |
| 13509 | Photoninduced charge redistribution of graphene determined by edge structures in the infrared region. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 229, 117858. | 2.0 | 8 |
| 13510 | Au ₂ Si ₂₀ : a honeycomb-shaped structure with short Au~Au single bond at the centre coordinated by twelve Si ₅ pentagons and reinforced by strong Au~Si interactions and aromaticity. <i>Molecular Physics</i> , 2020, 118, e1692152. | 0.8 | 4 |
| 13511 | On the Interplay between Charge-Shift Bonding and Halogen Bonding. <i>ChemPhysChem</i> , 2020, 21, 240-250. | 1.0 | 18 |
| 13512 | Chemical pathways for the formation of benzofuran and dibenzofuran in combustion. <i>Combustion and Flame</i> , 2020, 212, 216-233. | 2.8 | 17 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13513 | Investigating molecular mechanism for the stability of ternary systems containing cetrimide, fatty alcohol and water by using computer simulation. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 95, 107500. | 1.3 | 5 |
| 13514 | Assessing the Calculation of Exchange Coupling Constants and Spin Crossover Gaps Using the Approximate Projection Model To Improve Density Functional Calculations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 154-163. | 2.3 | 6 |
| 13515 | Unveiling the Photophysical Properties of Boron-dipyrromethene Dyes Using a New Accurate Excited State Coupled Cluster Method. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 564-575. | 2.3 | 64 |
| 13516 | QSAR/QSPR models based on quantum chemistry for risk assessment of pesticides according to current European legislation. <i>SAR and QSAR in Environmental Research</i> , 2020, 31, 49-72. | 1.0 | 27 |
| 13517 | Ligand-Mediated Regioselective Rhodium-Catalyzed Benzotriazole-Allene Coupling: Mechanistic Exploration and Quantum Chemical Analysis. <i>Chemistry - A European Journal</i> , 2020, 26, 2342-2348. | 1.7 | 16 |
| 13518 | Ammonia gas adsorption study on graphene oxide based sensing device under different humidity conditions. <i>Materials Chemistry and Physics</i> , 2020, 242, 122485. | 2.0 | 24 |
| 13519 | A novel 3-((5-methylpyridin-2-yl)amino)isobenzofuran-1(3H)-one: Molecular structure describe, X-ray diffractions and DFT calculations, antioxidant activity, DNA binding and molecular docking studies. <i>Journal of Molecular Structure</i> , 2020, 1205, 127585. | 1.8 | 17 |
| 13520 | Effect of molecular backbone structure on vapor phase coupling reaction between diiso(thio)cyanates with diamines, diols, and dithiols. <i>Progress in Organic Coatings</i> , 2020, 140, 105509. | 1.9 | 4 |
| 13521 | Self-Consistent Implementation of Hybrid Functionals with Local Range Separation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 953-963. | 2.3 | 19 |
| 13522 | Elucidating the Role of Catalyst Steric and Electronic Effects in Controlling the Synthesis of π -Conjugated Polymers. <i>Macromolecules</i> , 2020, 53, 138-148. | 2.2 | 15 |
| 13523 | Electroactivated alkylation of amines with alcohols <i>via</i> both direct and indirect borrowing hydrogen mechanisms. <i>Green Chemistry</i> , 2020, 22, 860-869. | 4.6 | 8 |
| 13524 | Hole Transfer in Open Carbynes. <i>Materials</i> , 2020, 13, 3979. | 1.3 | 3 |
| 13525 | Electrochemical, theoretical and surface physicochemical studies of the alkaline copper corrosion inhibition by newly synthesized molecular complexes of benzenediamine and tetraamine with π acceptor. <i>Journal of Molecular Liquids</i> , 2020, 320, 114386. | 2.3 | 8 |
| 13526 | Cocrystallization of 2,4-Diamino-6-phenyl-1,3,5-triazine with β -(phenylthio)propionic acid: Crystal structure, Hirshfeld surface, DFT studies and molecular docking. <i>Chemical Data Collections</i> , 2020, 29, 100520. | 1.1 | 1 |
| 13527 | The pyrrole-water complex: Multidimensional large amplitude dynamics and rotational spectra of its ^{13}C isotopologues. <i>Journal of Molecular Spectroscopy</i> , 2020, 374, 111381. | 0.4 | 5 |
| 13528 | Solvent and Anion Effects on the Electrochemistry of Manganese Dipyrrin-Bisphenols. <i>Inorganic Chemistry</i> , 2020, 59, 15913-15927. | 1.9 | 5 |
| 13529 | Synthesis, Structure, Dynamics, and Enantioface-Selective η^3 -Benzyl Coordination in the Chiral Rhodium Complexes $\text{Rh}(\text{diphos}^*)(\eta^3\text{-CH}_2\text{Ph})$. <i>Organometallics</i> , 2020, 39, 3802-3816. | 1.1 | 3 |
| 13530 | Cyclodextrin Porous Liquid Materials for Efficient Chiral Recognition and Separation of Nucleosides. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 45916-45928. | 4.0 | 50 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 13531 | Metallophthalocyanines in a ternary photoactive layer (P3HT:MPc:PC ₇₀ BM) for bulk heterojunction solar cells. <i>Materials Advances</i> , 2020, 1, 3058-3072. | 2.6 | 2 |
| 13532 | The effect of the degree of substitution on the solubility of cellulose acetoacetates in water: A molecular dynamics simulation and density functional theory study. <i>Carbohydrate Research</i> , 2020, 496, 108134. | 1.1 | 9 |
| 13533 | Machine Learning Predicts Degree of Aromaticity from Structural Fingerprints. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4560-4568. | 2.5 | 3 |
| 13534 | Perturbation of Pyridinium CVP Spectra by N ₂ and H ₂ Tags: An Experimental and BOMD Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8519-8528. | 1.1 | 5 |
| 13535 | Evaluation of Single-Reference DFT-Based Approaches for the Calculation of Spectroscopic Signatures of Excited States Involved in Singlet Fission. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8446-8460. | 1.1 | 10 |
| 13536 | Unequivocal structure confirmation of a breifussin analog by anisotropic NMR measurements. <i>Chemical Science</i> , 2020, 11, 12081-12088. | 3.7 | 9 |
| 13537 | Theoretical study on the catalytic mechanism of human deoxyhypusine hydroxylase. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22736-22745. | 1.3 | 6 |
| 13538 | OrbNet: Deep learning for quantum chemistry using symmetry-adapted atomic-orbital features. <i>Journal of Chemical Physics</i> , 2020, 153, 124111. | 1.2 | 153 |
| 13539 | Halogen-bonded haloamine trimers – modelling the X ₃ synthon. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 21938-21946. | 1.3 | 6 |
| 13540 | PyVibMS: a PyMOL plugin for visualizing vibrations in molecules and solids. <i>Journal of Molecular Modeling</i> , 2020, 26, 290. | 0.8 | 14 |
| 13541 | Low-Valence Anionic $\hat{\text{I}}\text{-Diimine Iron Complexes: Synthesis, Characterization, and Catalytic Hydroboration Studies. Inorganic Chemistry, 2020, 59, 16035-16052.$ | 1.9 | 23 |
| 13542 | Hydrogenative Metathesis of Enynes via Piano-Stool Ruthenium Carbene Complexes Formed by Alkyne gem-Hydrogenation. <i>Journal of the American Chemical Society</i> , 2020, 142, 18541-18553. | 6.6 | 30 |
| 13543 | Configuration Flipping in Distal Pocket of Multidrug Transporter MexB Impacts the Efflux Inhibitory Mechanism. <i>ChemPhysChem</i> , 2020, 21, 2516-2524. | 1.0 | 8 |
| 13544 | Spin-gapless semiconductors for future spintronics and electronics. <i>Physics Reports</i> , 2020, 888, 1-57. | 10.3 | 64 |
| 13545 | Multicenter electron-sharing $\hat{\text{I}}\text{-bonding in the AgFe(CO)}_4^{\text{+}}$ complex. <i>Dalton Transactions</i> , 2020, 49, 15256-15266. | 1.6 | 5 |
| 13546 | Questioning the Affinity of Electrophilic Astatine for Sulfur-containing Compounds: Unexpected Bindings Revealed. <i>Inorganic Chemistry</i> , 2020, 59, 13923-13932. | 1.9 | 15 |
| 13547 | Mechanism of the highly effective peptide bond hydrolysis by MOF-808 catalyst under biologically relevant conditions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25136-25145. | 1.3 | 22 |
| 13548 | van der Waals potential: an important complement to molecular electrostatic potential in studying intermolecular interactions. <i>Journal of Molecular Modeling</i> , 2020, 26, 315. | 0.8 | 126 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13549 | Novel benzothiazole half-squaraines: model chromophores to study dye-TiO ₂ interactions in dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2020, 8, 22191-22205. | 5.2 | 4 |
| 13550 | Calculation of magnetic properties with density functional approximations including rung 3.5 ingredients. <i>Journal of Chemical Physics</i> , 2020, 153, 164101. | 1.2 | 1 |
| 13551 | New Pt(II) complexes with 3 TM -methyl tetrahydro-4H-thiopyranspiro-5 TM -hydantoin: synthesis, theoretical and cytotoxic investigation. <i>Medicinal Chemistry Research</i> , 2020, 29, 2218-2223. | 1.1 | 1 |
| 13552 | Unsaturated binuclear homoleptic nickel carbonyl anions Ni ₂ (CO) _n ⁺ ($n = 4-6$) featuring double three-center two-electron Ni-C-Ni bonds. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 23773-23784. | 1.3 | 4 |
| 13553 | Toward the Formation of N-Heterocyclic-Carbene-Protected Gold Clusters of Various Nuclearities. A Comparison with Their Phosphine-Protected Analogues from Density Functional Theory Calculations. <i>Inorganic Chemistry</i> , 2020, 59, 15240-15249. | 1.9 | 14 |
| 13554 | High temperature pure carbon nanoparticle formation: Validation of AIREBO and ReaxFF reactive molecular dynamics. <i>Carbon</i> , 2020, 170, 606-620. | 5.4 | 51 |
| 13555 | Boron extraction from lithium-rich brine using mixed alcohols. <i>Hydrometallurgy</i> , 2020, 197, 105477. | 1.8 | 15 |
| 13556 | Efforts towards Rh(II)-catalyzed N-alkoxyazomethine ylide generation: Disparate reactivities of O-tethered α -diazo keto and β -ketoester oximes. <i>Tetrahedron</i> , 2020, 76, 131501. | 1.0 | 1 |
| 13557 | Mechanistic Insights into the Synthesis of Telluride Colloidal Quantum Dots with Trioctylphosphine-Tellurium. <i>ChemistrySelect</i> , 2020, 5, 11896-11900. | 0.7 | 7 |
| 13558 | Five-coordinate transition metal complexes and the value of $\langle i \rangle$, $\langle i \rangle_{5}$: observations and caveats. <i>Dalton Transactions</i> , 2020, 49, 14798-14806. | 1.6 | 59 |
| 13559 | Probing a Silent Metal: A Combined X-ray Absorption and Emission Spectroscopic Study of Biologically Relevant Zinc Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 13551-13560. | 1.9 | 16 |
| 13560 | Elucidating the Improved Electrolyte Stability with Novel Benzimidazole Salt on the Li Anode Surface: Insights into Interfacial Reactions. <i>Journal of Physical Chemistry C</i> , 2020, 124, 23523-23531. | 1.5 | 8 |
| 13561 | Dual redox mediators accelerate the electrochemical kinetics of lithium-sulfur batteries. <i>Nature Communications</i> , 2020, 11, 5215. | 5.8 | 113 |
| 13562 | The Chemistry of Acylgermanes: Triacylgermenolates Represent Valuable Building Blocks for the Synthesis of a Variety of Germanium-Based Photoinitiators. <i>Inorganic Chemistry</i> , 2020, 59, 15204-15217. | 1.9 | 18 |
| 13563 | Converging Interests: Chemoinformatics, History, and Bibliometrics. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5870-5872. | 2.5 | 2 |
| 13564 | Density Functional Theory Investigation of As(III) S-Adenosylmethionine Methyltransferase. <i>ACS Omega</i> , 2020, 5, 21000-21006. | 1.6 | 0 |
| 13565 | Bis-Ferrocenyl-Pyridinediimine Trinuclear Mixed-Valent Complexes with Metal-Binding Dependent Electronic Coupling: Synthesis, Structures, and Redox-Spectroscopic Characterization. <i>Journal of the American Chemical Society</i> , 2020, 142, 18715-18729. | 6.6 | 19 |
| 13566 | Systematic comparison and cross-validation of fixed-node diffusion Monte Carlo and phaseless auxiliary-field quantum Monte Carlo in solids. <i>Physical Review B</i> , 2020, 102, . | 1.1 | 13 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13567 | Proton inversion tunneling in the rotational spectrum of acetone cyanohydrin. <i>Journal of Molecular Spectroscopy</i> , 2020, 373, 111372. | 0.4 | 7 |
| 13568 | A DFT Study on the Cyclization-Mechanism during Process of Thermal Vacuum Degradation for Poly(dimethylsiloxanes). <i>Polymer Degradation and Stability</i> , 2020, 182, 109367. | 2.7 | 7 |
| 13569 | Highly Efficient Conversion of Ketazines to Pyrazoline Derivatives Catalyzed by FeCl ₃ . <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 18748-18755. | 1.8 | 6 |
| 13570 | Photosynthesis of a Dihydroimidazopyridine Chelate Shines Light on the Reactions of a Photoactivated Iron(III) Complex with O ₂ . <i>Inorganic Chemistry</i> , 2020, 59, 16281-16290. | 1.9 | 5 |
| 13571 | Chemical Potential and Thermodynamic Properties of Self-Assembled Monolayers: A Method of External Fields in a Monte Carlo Simulation. <i>Journal of Physical Chemistry C</i> , 2020, 124, 22447-22458. | 1.5 | 7 |
| 13572 | N-Activated 1,3-Benzoxazine Monomer as a Key Agent in Polybenzoxazine Synthesis. <i>Macromolecules</i> , 2020, 53, 8202-8215. | 2.2 | 10 |
| 13573 | Potential for Ladderane (Bio)synthesis from Oligo-Cyclopropane Precursors. <i>ACS Omega</i> , 2020, 5, 26134-26140. | 1.6 | 3 |
| 13574 | Gas-liquid water interface engineered exceptional photoconversion of fatty acids to olefins. <i>Green Chemistry</i> , 2020, 22, 7848-7857. | 4.6 | 4 |
| 13575 | Proving the Dual Electronic Structure of Charged Metal-Molecule Interfaces: Surface-Enhanced Raman Scattering of Cyanide Adsorbed on a Nanostructured Silver Electrode. <i>Journal of Physical Chemistry C</i> , 2020, 124, 17632-17639. | 1.5 | 6 |
| 13576 | Unmasking Static Correlation Error in Hybrid Kohn-Sham Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5432-5440. | 2.3 | 25 |
| 13577 | Computational Study for the Reaction Mechanism of <i>N</i> -Hydroxyphthalimide-Catalyzed Oxidative Cleavage of Alkenes. <i>Journal of Organic Chemistry</i> , 2020, 85, 10136-10142. | 1.7 | 5 |
| 13578 | Catalytic Mechanism of Human Aldehyde Oxidase. <i>ACS Catalysis</i> , 2020, 10, 9276-9286. | 5.5 | 20 |
| 13579 | Spin controlled surface chemistry: alkyl desorption from Si(100)-2 \times 1 by nonadiabatic hydrogen elimination. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16641-16647. | 1.3 | 2 |
| 13580 | Benchmark and parameter tuning of hybrid functionals for fast calculation of excitation energies of AlEgens. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 18035-18039. | 1.3 | 11 |
| 13581 | Hole-hole Tamm-Dancoff-approximated density functional theory: A highly efficient electronic structure method incorporating dynamic and static correlation. <i>Journal of Chemical Physics</i> , 2020, 153, 024110. | 1.2 | 34 |
| 13582 | Some useful correlations for H-bonded systems. <i>Molecular Crystals and Liquid Crystals</i> , 2020, 696, 15-28. | 0.4 | 6 |
| 13583 | Chalcogen-mercury bond formation and disruption in model Rabenstein's reactions: A computational analysis. <i>Journal of Computational Chemistry</i> , 2020, 41, 2045-2054. | 1.5 | 13 |
| 13584 | Atmospheric Chemistry of Methyl Isocyanide—An Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6562-6571. | 1.1 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 13585 | S 2p and P 2p Core Level Spectroscopy of PPT Ambipolar Material and Its Building Block Moieties. <i>Journal of Physical Chemistry C</i> , 2020, 124, 14510-14520. | 1.5 | 3 |
| 13586 | Compression of curium pyrrolidine-dithiocarbamate enhances covalency. <i>Nature</i> , 2020, 583, 396-399. | 13.7 | 34 |
| 13587 | Experimental and theoretical studies of 2-Mercaptobenzothiazole with 2-Bromomethylmesitylene and 1,4-Bis(bromomethyl)durene. <i>Journal of Molecular Structure</i> , 2020, 1222, 128894. | 1.8 | 7 |
| 13588 | Electrostatic Field-Induced Oscillator Strength Focusing in Molecules. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6376-6388. | 1.2 | 5 |
| 13589 | Determination of the pKa Values of trans-Resveratrol, a Triphenolic Stilbene, by Singular Value Decomposition. Comparison with Theory. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6294-6302. | 1.1 | 11 |
| 13590 | Investigation of the role of terminal ligands in magnetic relaxation in a series of dinuclear dysprosium complexes. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 3352-3363. | 3.0 | 20 |
| 13591 | Gas-Phase Hydration of Perillaldehyde Investigated by Microwave Spectroscopy Assisted by Computational Chemistry. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6511-6520. | 1.1 | 5 |
| 13592 | Real-Space Approach to the Reaction Force: Understanding the Origin of Synchronicity/Nonsynchronicity in Multibond Chemical Reactions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1959-1972. | 1.1 | 12 |
| 13593 | Insights into the Assembly of the Pseudogemini Surfactant at the Oil/Water Interface: A Molecular Simulation Study. <i>Langmuir</i> , 2020, 36, 1839-1847. | 1.6 | 20 |
| 13594 | Low-cost electrochemical detection of L-tyrosine using an rGO@Cu modified pencil graphite electrode and its surface orientation on a Ag electrode using an <i>ex situ</i> spectroelectrochemical method. <i>RSC Advances</i> , 2020, 10, 22871-22880. | 1.7 | 24 |
| 13595 | Rearrangement of <i>o</i> -(pivaloylamino)methylbenzaldehydes: an experimental and computational study. <i>Beilstein Journal of Organic Chemistry</i> , 2020, 16, 1636-1648. | 1.3 | 2 |
| 13596 | Theoretical study of propylene epoxidation heterogeneous-homogeneous mechanism over MoO _x / SiO ₂ catalyst. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26328. | 1.0 | 2 |
| 13597 | Density Functional Theories and Coordination Chemistry. , 2020, , . | | 2 |
| 13598 | Theoretical study of selective hydrogenolysis of methyl vinyl carbinol over Au-Ni bimetallic catalyst: Toward constructing a working hypothesis for the role of dichloroethane solvent and perimeter sites. <i>Chemical Physics Letters</i> , 2020, 754, 137773. | 1.2 | 1 |
| 13599 | Critical evaluation of anharmonicity and configurational averaging in QM/MM modelling of equilibrium isotope effects. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16267-16276. | 1.3 | 3 |
| 13600 | Mechanism and Origins of Product Selectivity of Au-Catalyzed Coupling Benzisoxazoles with Ynamides: A Computational Study. <i>ChemCatChem</i> , 2020, 12, 5276-5283. | 1.8 | 4 |
| 13601 | Solvent influence on molecular interactions in the bulk of fluorene copolymer films. <i>RSC Advances</i> , 2020, 10, 20772-20777. | 1.7 | 3 |
| 13602 | A Potential Inhibition Process of Ricin Protein with the flavonoids Quercetin and Epigallocatechin Gallate. A Quantum-Chemical and Molecular Docking Study. <i>Processes</i> , 2020, 8, 1393. | 1.3 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13603 | Overlap-Driven Splitting of Triplet Pairs in Singlet Fission. <i>Journal of the American Chemical Society</i> , 2020, 142, 20040-20047. | 6.6 | 26 |
| 13604 | Generalizing Double-Hybrid Density Functionals: Impact of Higher-Order Perturbation Terms. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7413-7430. | 2.3 | 12 |
| 13605 | Theoretical Insights into Ester-Directed Reactions between Propiolates with 1,2-Benzisoxazoles by Au(I) Catalyst: [4 + 2]-Annulation versus Michael-Type Products. <i>Organometallics</i> , 2020, 39, 4061-4068. | 1.1 | 4 |
| 13606 | NeoR, a near-infrared absorbing rhodopsin. <i>Nature Communications</i> , 2020, 11, 5682. | 5.8 | 45 |
| 13607 | A Computational Study on the Redox Reactions of Ammonia and Methylamine with Nitrogen Tetroxide. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9923-9932. | 1.1 | 3 |
| 13608 | Modelling the structural and reactivity landscapes of tucatinib with special reference to its wavefunction-dependent properties and screening for potential antiviral activity. <i>Journal of Molecular Modeling</i> , 2020, 26, 341. | 0.8 | 35 |
| 13609 | Assessing Zethrene Derivatives as Singlet Fission Candidates Based on Multiple Descriptors. <i>Journal of Physical Chemistry C</i> , 2020, 124, 26134-26143. | 1.5 | 10 |
| 13610 | Self-Consistent Calculation of the Localized Orbital Scaling Correction for Correct Electron Densities and Energy-Level Alignments in Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 10269-10277. | 2.1 | 18 |
| 13611 | Probing the tautomerization of disilenes and disilabenzenes with their isomeric silylenes: significant substituent, aromaticity and base effects. <i>Dalton Transactions</i> , 2020, 49, 17341-17349. | 1.6 | 2 |
| 13612 | Chiral Polyurea from Tartaric Acid Derived and Lysine Backbone: A Synthetic and Computational Study. <i>ChemistrySelect</i> , 2020, 5, 13358-13369. | 0.7 | 0 |
| 13613 | Stabilities, Electronic Structures, and Bonding Properties of Iron Complexes (E 1 E 2)Fe(CO) 2 (CNAr) Tj ETQq 0 0 0 rgBT /Overlock 10 TF | 0.9 | 2 |
| 13614 | Machine Learning K-Means Clustering Algorithm for Interpolative Separable Density Fitting to Accelerate Hybrid Functional Calculations with Numerical Atomic Orbitals. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10066-10074. | 1.1 | 35 |
| 13615 | Surface Hopping Dynamics for Azobenzene Photoisomerization: Effects of Packing Density on Surfaces, Fluorination, and Excitation Wavelength. <i>Journal of Physical Chemistry C</i> , 2020, 124, 26287-26295. | 1.5 | 7 |
| 13616 | Photorearrangement of [8]-2,6-Pyridinophane <i>N</i> -Oxide. <i>Journal of the American Chemical Society</i> , 2020, 142, 20717-20724. | 6.6 | 5 |
| 13617 | Thiocoumarin Caged Nucleotides: Synthetic Access and Their Photophysical Properties. <i>Molecules</i> , 2020, 25, 5325. | 1.7 | 7 |
| 13618 | Quantum Monte Carlo benchmarking of large noncovalent complexes in the L7 benchmark set. <i>Journal of Chemical Physics</i> , 2020, 153, 194113. | 1.2 | 14 |
| 13619 | Essential role of accessory subunit LYRM6 in the mechanism of mitochondrial complex I. <i>Nature Communications</i> , 2020, 11, 6008. | 5.8 | 25 |
| 13620 | On the synergy of matrix-isolation infrared spectroscopy and vibrational configuration interaction computations. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 174. | 0.5 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13621 | Examining the Spin State and Redox Chemistry of Ni(Diimine) Catalysts during the Synthesis of π -Conjugated Polymers. <i>Macromolecular Chemistry and Physics</i> , 2020, 221, 2000321. | 1.1 | 5 |
| 13622 | Computational Studies on the Mechanism and Origin of the Different Regioselectivities of Manganese Porphyrin-Catalyzed C-H Bond Hydroxylation and Amidation of Equilenin Acetate. <i>Journal of Organic Chemistry</i> , 2020, 85, 14879-14889. | 1.7 | 17 |
| 13623 | A Not Obvious Correlation Between the Structure of Green Fluorescent Protein Chromophore Pocket and Hydrogen Bond Dynamics: A Choreography From ab initio Molecular Dynamics. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 569990. | 1.6 | 23 |
| 13624 | Reactivity of arsenoplatin complex versus water and thiocyanate: a DFT benchmark study. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1. | 0.5 | 19 |
| 13625 | Simulation of vibrationally resolved absorption spectra of neutral and cationic polyaromatic hydrocarbons. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1. | 0.5 | 4 |
| 13626 | Electrochemical and Solvent-Mediated Visible-Near-Infrared Spectroscopic Switching of Benzoselenadiazole Fluorophores. <i>Chemistry - A European Journal</i> , 2020, 26, 17416-17427. | 1.7 | 9 |
| 13627 | Synthesis of Novel Biocompatible Thienopyrimidine Chromophores with Aggregation-Induced Emission Sensitive to Molecular Aggregation. <i>ACS Omega</i> , 2020, 5, 29988-30000. | 1.6 | 15 |
| 13628 | Theoretical Design of Dithienopicenocarbazole-Based Molecules by Molecular Engineering of Terminal Units Toward Promising Non-fullerene Acceptors. <i>Frontiers in Chemistry</i> , 2020, 8, 580252. | 1.8 | 7 |
| 13629 | Polyfuran-based chemical sensors: Identification of promising derivatives via DFT calculations and fully atomistic reactive molecular dynamics. <i>European Polymer Journal</i> , 2020, 141, 110085. | 2.6 | 14 |
| 13630 | SCC-DFTB Parameters for Fe-C Interactions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9674-9682. | 1.1 | 3 |
| 13631 | A Two-Step Catalytic Cycle for the Acceptorless Dehydrogenation of Ethane by Group 10 Metal Complexes: Role of the Metal in Reactivity and Selectivity. <i>Organometallics</i> , 2020, 39, 4027-4036. | 1.1 | 5 |
| 13632 | Investigation of the <i>cis</i> and <i>trans</i> structures and isomerization of oligoprolines by using Raman spectroscopy and density functional theory calculations: solute-solvent interactions and effects of terminal positively charged amino acid residues. <i>RSC Advances</i> , 2020, 10, 34493-34500. | 1.7 | 2 |
| 13633 | Predicting Bond Dissociation Energies and Bond Lengths of Coordinatively Unsaturated Vanadium-Ligand Bonds. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9757-9770. | 1.1 | 5 |
| 13634 | New Aspects of the Airglow Problem and Reactivity of the Dioxygen Quintet $O_2(^5\Sigma_g^-)$ State in the MLT Region as Predicted by DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9638-9655. | 1.1 | 7 |
| 13635 | Circumventing Scaling Relations in Oxygen Electrochemistry Using Metal-Organic Frameworks. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 10029-10036. | 2.1 | 32 |
| 13636 | Participation of Phosphorylated Analogues of Nitroethene in Diels-Alder Reactions with Anthracene: A Molecular Electron Density Theory Study and Mechanistic Aspect. <i>Organics</i> , 2020, 1, 36-48. | 0.6 | 13 |
| 13637 | Quantum algorithm for simulating molecular vibrational excitations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25528-25537. | 1.3 | 16 |
| 13638 | Relationship between molecular charge distribution and wettability reversal efficiency of cationic surfactants on calcite surfaces. <i>Journal of Molecular Liquids</i> , 2020, 318, 114009. | 2.3 | 13 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13639 | Ultrafast Nonradiative Decay of a Dipolar Plasmon-like State in Naphthalene. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9729-9737. | 1.1 | 4 |
| 13640 | Enantioselectivity-Evaluation of Chiral Copper(II) Complexes Coordinated by Novel Chiral Tetradentate Ligands for Free Amino Acids by Mass Spectrometry Coupled With the Isotopically Labeled Enantiomer Method. <i>Frontiers in Chemistry</i> , 2020, 8, 598598. | 1.8 | 4 |
| 13641 | Combining EXAFS and Computer Simulations to Refine the Structural Description of Actinyls in Water. <i>Molecules</i> , 2020, 25, 5250. | 1.7 | 2 |
| 13642 | Laurdan and Di-4-ANEPPDHQ Influence the Properties of Lipid Membranes: A Classical Molecular Dynamics and Fluorescence Study. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11419-11430. | 1.2 | 20 |
| 13643 | A High-Performance Magnesium Triflate-based Electrolyte for Rechargeable Magnesium Batteries. <i>Cell Reports Physical Science</i> , 2020, 1, 100265. | 2.8 | 48 |
| 13644 | Combined Computational and Experimental Investigation on the Nature of Hydrated Iodoplumbate Complexes: Insights into the Dual Role of Water in Perovskite Precursor Solutions. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11481-11490. | 1.2 | 21 |
| 13645 | Conformational potential energy surfaces and cationic structure of 3,4-dihydro-2 <i>H</i> -pyran by VUV-MATI spectroscopy and Franck-Condon fitting. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27673-27680. | 1.3 | 3 |
| 13646 | New 1,3,4-Oxadiazole Derivatives of Pyridothiazine-1,1-Dioxide with Anti-Inflammatory Activity. <i>International Journal of Molecular Sciences</i> , 2020, 21, 9122. | 1.8 | 21 |
| 13647 | AMnAs ₃ S ₆ (A = Cs, Rb): Phase-Matchable Infrared Nonlinear Optical Functional Motif [As ₃ S ₆] ³⁻ Obtained via Surfactant-Assisted Thermal Method. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 53950-53956. | 4.0 | 25 |
| 13648 | A Review of Density Functional Models for the Description of Fe(II) Spin-Crossover Complexes. <i>Molecules</i> , 2020, 25, 5176. | 1.7 | 8 |
| 13649 | On the connection between probability density analysis, QTAIM, and VB theory. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25892-25903. | 1.3 | 13 |
| 13650 | Investigation of vacuum ultraviolet photoionization of methylcyclohexane in energy region of 9~15.5 eV. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 296-302. | 0.6 | 1 |
| 13651 | Theoretical analysis of an anion- I^- complex: $\text{I}^- \cdots \text{C}_6\text{F}_6$. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 285-290. | 0.6 | 3 |
| 13652 | Crystal Structure and Mechanistic Molecular Modeling Studies of Mycobacterium tuberculosis Diterpene Cyclase Rv3377c. <i>Biochemistry</i> , 2020, 59, 4507-4515. | 1.2 | 6 |
| 13653 | Visible-Light Photoredox-Catalyzed Remote Difunctionalizing Carboxylation of Unactivated Alkenes with CO ₂ . <i>Angewandte Chemie</i> , 2020, 132, 21307-21314. | 1.6 | 21 |
| 13654 | Crystal Structures and Fluorescence Spectroscopic Properties of a Series of I^{\pm} - $\text{Di}(4\text{-pyridyl})$ polyenes: Effect of Aggregation-Induced Emission. <i>ChemPlusChem</i> , 2020, 85, 1968-1980. | 1.3 | 3 |
| 13655 | Pyrolyzed pencil graphite coated cellulose paper as an interlayer: An effective approach for high-performance lithium-sulfur battery. <i>Applied Surface Science</i> , 2020, 533, 147483. | 3.1 | 30 |
| 13656 | Time-dependent density functional theory study of the X-ray emission spectroscopy of amino acids and proteins. <i>Chemical Physics Letters</i> , 2020, 757, 137860. | 1.2 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 13657 | Selective hydrogenation of acetylene catalyzed by nickel and nitrogen-doped C34: A density functional theory study. <i>Chemical Physics Letters</i> , 2020, 757, 137871. | 1.2 | 4 |
| 13658 | Molecular adsorption studies of benzidine on novel Kagome antimonene nanosheets - Insights based on first-principles DFT calculations. <i>Journal of Molecular Liquids</i> , 2020, 318, 113972. | 2.3 | 18 |
| 13659 | Tailored β -diketones as effective surface passivation for solution processed zinc oxide thin film transistors. <i>Organic Electronics</i> , 2020, 86, 105906. | 1.4 | 1 |
| 13660 | Benchmark Study of Electrochemical Redox Potentials Calculated with Semiempirical and DFT Methods. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7166-7176. | 1.1 | 45 |
| 13661 | Lewis Base/Acid Coordination Stabilizes Planar σ -Aromatic Si ₆ /P ₆ . <i>Organometallics</i> , 2020, 39, 2951-2955. | 1.1 | 2 |
| 13662 | Observation of inhomogeneous plasmonic field distribution in a nanocavity. <i>Nature Nanotechnology</i> , 2020, 15, 922-926. | 15.6 | 62 |
| 13663 | Globally stabilized bent carbon-carbon triple bond by hydrogen-free inorganic-metallic scaffolding Al ₄ F ₆ . <i>RSC Advances</i> , 2020, 10, 25275-25280. | 1.7 | 0 |
| 13664 | Photophysical characterization of new osmium (II) photocatalysts for hydrohalic acid splitting. <i>Journal of Chemical Physics</i> , 2020, 153, 054307. | 1.2 | 5 |
| 13665 | A thorough theoretical exploration of the effect mechanism of Fe on HCN heterogeneous formation from nitrogen-containing char. <i>Fuel</i> , 2020, 280, 118662. | 3.4 | 29 |
| 13666 | Variation of the Fine-Structure Constant in Model Systems for Singlet Fission. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6682-6687. | 1.1 | 1 |
| 13667 | A new ionone derivative from <i>Lycium intricatum</i> Boiss. (Solanaceae). <i>Natural Product Research</i> , 2022, 36, 687-694. | 1.0 | 3 |
| 13668 | Insights into the binding of dorzagliatin with glucokinase: A molecular dynamics simulation. <i>Journal of Theoretical and Computational Chemistry</i> , 2020, 19, 2050027. | 1.8 | 9 |
| 13669 | Microscopic mechanism for effect of sodium on NO heterogeneous reduction by char. <i>Journal of Fuel Chemistry and Technology</i> , 2020, 48, 663-673. | 0.9 | 16 |
| 13670 | Reactions of Tricyclo[4.1.0.0 ^{2,7}]heptane and 1-Methyltricyclo[4.1.0.0 ^{2,7}]heptane with 2-Bromoethanesulfonyl Bromide. <i>Russian Journal of Organic Chemistry</i> , 2020, 56, 1014-1022. | 0.3 | 0 |
| 13671 | Understanding a Thermoemissive ESIPT-Based Solid-State Off-On Switch as a Dual-Channel Chemosensor in Solid and Solution Phases: Detailed Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 18181-18193. | 1.5 | 15 |
| 13672 | Applications of Quantum Chemistry in Pharmaceutical Process Development: Current State and Opportunities. <i>Organic Process Research and Development</i> , 2020, 24, 1496-1507. | 1.3 | 25 |
| 13673 | Density functional theory calculations of the effect (CH ₂ , CH ₃ , NH ₃ , NH ₂ , OH, CN, NO ₂) subgroups on the electronic structure of biphenyl molecule. <i>IOP Conference Series: Materials Science and Engineering</i> , 2020, 871, 012067. | 0.3 | 0 |
| 13674 | Exchange-correlation functionals for band gaps of solids: benchmark, reparametrization and machine learning. <i>Npj Computational Materials</i> , 2020, 6, . | 3.5 | 156 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13675 | Gasâ€Phase Models for the Nickelâ€and Palladiumâ€Catalyzed Deoxygenation of Fatty Acids. <i>ChemCatChem</i> , 2020, 12, 5476-5485. | 1.8 | 6 |
| 13676 | Cyclic Carbonate Formation from Epoxides and CO ₂ Catalyzed by Sustainable Alkali Halideâ€Glycol Complexes: A DFT Study to Elucidate Reaction Mechanism and Catalytic Activity. <i>ACS Omega</i> , 2020, 5, 18064-18072. | 1.6 | 20 |
| 13677 | Pentacyanoferrate(II) complex of pyridine-4- and pyrazine-2-hydroxamic acid as source of HNO: investigation of anti-tubercular and vasodilation activities. <i>Journal of Biological Inorganic Chemistry</i> , 2020, 25, 887-901. | 1.1 | 8 |
| 13678 | Structureâ€activity relationships in well-defined conjugated oligomer photocatalysts for hydrogen production from water. <i>Chemical Science</i> , 2020, 11, 8744-8756. | 3.7 | 41 |
| 13679 | Visibleâ€Light Photoredoxâ€Catalyzed Remote Difunctionalizing Carboxylation of Unactivated Alkenes with CO ₂ . <i>Angewandte Chemie - International Edition</i> , 2020, 59, 21121-21128. | 7.2 | 102 |
| 13680 | Diborane Concatenation Leads to New Planar Boron Chemistry. <i>ChemPhysChem</i> , 2020, 21, 2460-2467. | 1.0 | 17 |
| 13681 | The effect of additives (pyrazine, pyrazole and their derivatives) in the oxidation of 2-butanol with FeCl ₃ â€H ₂ O ₂ in aqueous solutions. <i>Catalysis Today</i> , 2021, 381, 163-170. | 2.2 | 5 |
| 13682 | Mechanistic Insight into the Catalytic NO Oxidation by the MIL-100 MOF Platform: Toward the Prediction of More Efficient Catalysts. <i>ACS Catalysis</i> , 2020, 10, 9445-9450. | 5.5 | 22 |
| 13683 | Beyond Solvent Exclusion: i-Motif Detecting Capability and an Alternative DNA Light-Switching Mechanism in a Ruthenium(II) Polypyridyl Complex. <i>Journal of the American Chemical Society</i> , 2020, 142, 13856-13866. | 6.6 | 23 |
| 13684 | Spiro-type host materials with rigidified skeletons for RGB phosphorescent OLEDs. <i>Journal of Materials Chemistry C</i> , 2020, 8, 12470-12477. | 2.7 | 13 |
| 13685 | Diastereodivergent aminocatalyzed spirocyclization strategies using 4-alkylideneisoxazol-5-ones and methyl vinyl ketones. <i>Organic Chemistry Frontiers</i> , 2020, 7, 3599-3607. | 2.3 | 11 |
| 13686 | Quasi-relativistic study of nuclear electric quadrupole coupling constants in chiral molecules containing heavy elements. <i>Molecular Physics</i> , 2020, 118, e1797199. | 0.8 | 2 |
| 13687 | Simple and Accurate Exchange Energy for Density Functional Theory. <i>Molecules</i> , 2020, 25, 3485. | 1.7 | 4 |
| 13688 | Transient species of esculetin produced in pulse radiolysis: experimental and quantum chemical investigations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 18573-18584. | 1.3 | 1 |
| 13689 | Dynamics of isobutane is a sensitive probe for framework breathing in MIL-53 (Al) MOF. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 18695-18702. | 1.3 | 8 |
| 13690 | Opto-Electronic properties of BN-ring insertions in Circumacenes: the case of Coronene and Ovalene. <i>Journal of Physics: Conference Series</i> , 2020, 1548, 012028. | 0.3 | 3 |
| 13691 | Dioxygen Binding to all 3d, 4d, and 5d Transition Metals from Coupledâ€Cluster Theory. <i>ChemPhysChem</i> , 2020, 21, 2173-2186. | 1.0 | 2 |
| 13692 | A Computational and Modeling Study of the Reaction Mechanism of <i>Staphylococcus aureus</i> Monoglycosyltransferase Reveals New Insights on the GT51 Family of Enzymes. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5513-5528. | 2.5 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13693 | Insights into the Regioselectivity of Hydroheteroarylation of Allylbenzene with Pyridine Catalyzed by Ni/AlMe ₃ with <i>N</i> -Heterocyclic Carbene: The Concerted Hydrogen Transfer Mechanism. <i>Journal of Organic Chemistry</i> , 2020, 85, 11340-11349. | 1.7 | 13 |
| 13694 | Regulation of Electronic Structure of Graphene Nanoribbon by Tuning Long-Range Dopant "Dopant Coupling at Distance of Tens of Nanometers. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 6907-6913. | 2.1 | 5 |
| 13695 | C,N-chelated diaminocarbene platinum(II) complexes derived from 3,4-diaryl-1H-pyrrol-2,5-diimines and cis-dichlorobis(isonitrile)platinum(II): Synthesis, cytotoxicity, and catalytic activity in hydrosilylation reactions. <i>Journal of Organometallic Chemistry</i> , 2020, 923, 121435. | 0.8 | 11 |
| 13696 | Probing resonance effects in aromatic systems by nuclear quadrupole Coupling: Investigations of 3- and 4-chlorophenol by rotational spectroscopy. <i>Journal of Molecular Structure</i> , 2020, 1217, 128224. | 1.8 | 2 |
| 13697 | Quantum chemical prediction of the spectroscopic properties and ionic composition of the molten NaF-AlF ₃ salts. <i>Journal of Molecular Liquids</i> , 2020, 317, 113937. | 2.3 | 12 |
| 13698 | First-principles insight on interaction behavior of diethylbenzene and ethyltoluene on Γ -arsenene nanoring. <i>Materials Today Communications</i> , 2020, 25, 101476. | 0.9 | 3 |
| 13699 | Formation and desorption of nickel hexafluoroacetylacetonate Ni(hfac) ₂ on a nickel oxide surface in atomic layer etching processes. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2020, 38, . | 0.9 | 12 |
| 13700 | Large-scale comparison of 3d and 4d transition metal complexes illuminates the reduced effect of exchange on second-row spin-state energetics. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19326-19341. | 1.3 | 20 |
| 13701 | Conceptualization and Synthesis of the First Inositol (Decahydroxydecalin, DHD): In...silico Binding to β -Amyloid Protein. <i>Chemistry - A European Journal</i> , 2020, 26, 17005-17010. | 1.7 | 2 |
| 13702 | Revisiting immiscibility through DFT chemical descriptors. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1. | 0.5 | 1 |
| 13703 | Addressing the Hypervalent Model: A Straightforward Explanation of Traditionally Hypervalent Molecules. <i>Journal of Chemical Education</i> , 2020, 97, 3638-3646. | 1.1 | 10 |
| 13704 | Basis Set Extrapolations for Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5712-5722. | 2.3 | 13 |
| 13705 | Electrochemical oxidation of resorcinol: mechanistic insights from experimental and computational studies. <i>RSC Advances</i> , 2020, 10, 28454-28463. | 1.7 | 25 |
| 13706 | Ultra-High Stokes Shift in Polycyclic Chromeno[2,3- <i>b</i>]Indoles. <i>Polycyclic Aromatic Compounds</i> , 2022, 42, 1710-1727. | 1.4 | 3 |
| 13707 | Elastic electron scattering by tetramethylmethane, tetramethylsilane, and tetramethylgermane. <i>Physical Review A</i> , 2020, 102, . | 1.0 | 3 |
| 13708 | Nb(<i>i</i> -PrNPMe ₂) ₃ Fe(PMe ₃): A potential high reactivity heterobimetallic catalyst for acetylene cycloadditions. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5966. | 1.7 | 4 |
| 13709 | Benchmark study of density functionals for the insertions of olefin and polar monomers catalyzed by Γ -diimine palladium complexes. <i>Computational and Theoretical Chemistry</i> , 2020, 1187, 112942. | 1.1 | 3 |
| 13710 | Charge transfer via spin flip configuration interaction: Benchmarks and application to singlet fission. <i>Journal of Chemical Physics</i> , 2020, 153, 064109. | 1.2 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 13711 | A Boron Dipyrromethene-Based Fluorescence "OFF-ON"™ Probe for Sensitive and Selective Detection of Palladium(II) Ions and Its Application in Live Cell Imaging. <i>Chemistry - an Asian Journal</i> , 2020, 15, 4104-4112. | 1.7 | 14 |
| 13712 | One Electron Multiple Proton Transfer in Model Organic Donor-Acceptor Systems: Implications for High-Frequency EPR. <i>Applied Magnetic Resonance</i> , 2020, 51, 977-991. | 0.6 | 1 |
| 13713 | Theoretical spectroscopy of isotopically dilute water and hydrophobicity. <i>Journal of Chemical Physics</i> , 2020, 153, 094501. | 1.2 | 4 |
| 13714 | Non-precious-metal catalysts for alkaline water electrolysis: <i>operando</i> characterizations, theoretical calculations, and recent advances. <i>Chemical Society Reviews</i> , 2020, 49, 9154-9196. | 18.7 | 448 |
| 13715 | Mechanistic insights of selective syngas conversion over Zn grafted on ZSM-5 zeolite. <i>Catalysis Science and Technology</i> , 2020, 10, 8173-8181. | 2.1 | 6 |
| 13716 | Substituent-regulated mechanism on reaction Cp ₂ NbH ₃ (Cp = η^5 -C ₅ H ₅) with RCi ₂ CR (R = COOMe and Me). <i>Dalton Transactions</i> , 2020, 49, 15376-15384. | 1.6 | 0 |
| 13717 | The Non-innocent Role of Spin Traps in Monitoring Radical Formation in Copper-Catalyzed Reactions. <i>Applied Magnetic Resonance</i> , 2020, 51, 1529-1542. | 0.6 | 3 |
| 13718 | Adsorption studies on small toxic gases using silicane nanosheet as a chemi-resistive sensor "DFT method. <i>Computational and Theoretical Chemistry</i> , 2020, 1191, 113046. | 1.1 | 4 |
| 13719 | High-resolution vacuum ultraviolet absorption spectra of 2,3- and 2,5-dihydrofuran. <i>Journal of Chemical Physics</i> , 2020, 153, 134303. | 1.2 | 1 |
| 13720 | Production and Characterization of Molecular Dications: Experimental and Theoretical Efforts. <i>Molecules</i> , 2020, 25, 4157. | 1.7 | 9 |
| 13721 | Exploring ground and low-lying excited states for diquat, paraquat, and dipyrindyl isomers. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 402, 112817. | 2.0 | 9 |
| 13722 | Study of three new halogenated oxoquinolinecarbohydrazide N-phosphonate derivatives as corrosion inhibitor for mild steel in acid environment. <i>Surfaces and Interfaces</i> , 2020, 21, 100773. | 1.5 | 15 |
| 13723 | The diffusion of doxorubicin drug molecules in silica nanoslits is non-Gaussian, intermittent and anticorrelated. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27955-27965. | 1.3 | 55 |
| 13724 | DFT Study on the Mechanism of 4,4'-Bipyridine-Catalyzed Nitrobenzene Reduction by Diboron(4) Compounds. <i>Journal of Organic Chemistry</i> , 2020, 85, 13877-13885. | 1.7 | 10 |
| 13725 | Structural evolution from exohedral to endohedral geometries, dynamical fluxionality, and structural forms of medium-sized anionic and neutral Au ₂ Si _n (n = 8-20) clusters. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25606-25617. | 1.3 | 0 |
| 13726 | Analytic energy gradients of spin-adapted open-shell time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2020, 153, 164109. | 1.2 | 20 |
| 13727 | Fluorinated vs Nonfluorinated PR ₂ (biaryl) Ligands and Their [AuCl(L)] Complexes: Synthesis, X-ray Structures, and Computational Study of Weak Interactions. <i>Bond, No Bond, and Beyond. Inorganic Chemistry</i> , 2020, 59, 16599-16610. | 1.9 | 10 |
| 13728 | Highly Efficient Thermally Activated Delayed Fluorescence via an Unconjugated Donor-Acceptor System Realizing EQE of Over 30%. <i>Advanced Materials</i> , 2020, 32, e2003885. | 11.1 | 148 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13729 | Direct Hydroxylation of Methane. , 2020, , . | | 6 |
| 13730 | A combined experimental and DFT approach on free radical induced oxidations of kynurenic acid. <i>New Journal of Chemistry</i> , 2020, 44, 18858-18866. | 1.4 | 5 |
| 13731 | Metal-organic magnets with large coercivity and ordering temperatures up to 242Å°C. <i>Science</i> , 2020, 370, 587-592. | 6.0 | 91 |
| 13732 | Asparagine and Glutamine Side-Chains and Ladders in HET-s(218Å€289) Amyloid Fibrils Studied by Fast Magic-Angle Spinning NMR. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 582033. | 1.6 | 12 |
| 13733 | Spectroscopic (IR, Raman, UV, NMR) characterization and investigation of reactive properties of pyrazine-2-carboxamide by anti-bacterial, anti-mycobacterial, Fukui function, molecular docking and DFT calculations. <i>Chemical Data Collections</i> , 2020, 30, 100583. | 1.1 | 8 |
| 13734 | Microbial Cleavage of CÅ€F Bonds in Two C₆ Per- and Polyfluorinated Compounds via Reductive Defluorination. <i>Environmental Science & Technology</i> , 2020, 54, 14393-14402. | 4.6 | 73 |
| 13735 | Prediction of CO2 chemical absorption isotherms for ionic liquid design by DFT/COSMO-RS calculations. <i>Chemical Engineering Journal Advances</i> , 2020, 4, 100038. | 2.4 | 11 |
| 13736 | ESPÅ€ALIE Analysis as a Theoretical Tool for Identifying the Coordination Atoms of Possible Multisite Extractants: Validation and Prediction. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 14353-14364. | 3.2 | 7 |
| 13737 | Construction of amperometric biosensor modified with conducting polymer/carbon dots for the analysis of catechol. <i>Journal of Polymer Science</i> , 2020, 58, 3336-3348. | 2.0 | 18 |
| 13738 | Cumulene Wires Display Increasing Conductance with Increasing Length. <i>Nano Letters</i> , 2020, 20, 8415-8419. | 4.5 | 47 |
| 13739 | Decomposition pathway of C4F7N gas considering the participation of ions. <i>Journal of Applied Physics</i> , 2020, 128, . | 1.1 | 11 |
| 13740 | Exceptionally High OÅ€H Bond Dissociation Free Energy of a Dicopper(II) Î¼-Hydroxo Complex and Insights into the Geometric and Electronic Structure Origins Thereof. <i>Journal of the American Chemical Society</i> , 2020, 142, 16292-16312. | 6.6 | 10 |
| 13741 | Synthesis and Photophysical Properties of HexabenzocoroneneÅ€Tetrabenzoporphyrin Architectures. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 6352-6360. | 1.2 | 6 |
| 13742 | DFT<sc>Å€D4</sc> counterparts of leading <sc>metaÅ€</sc>generalizedÅ€gradient approximation and hybrid density functionals for energetics and geometries. <i>Journal of Computational Chemistry</i> , 2020, 41, 2562-2572. | 1.5 | 61 |
| 13743 | Triarylverdazyl radicals as promising redox-active components of rechargeable organic batteries. <i>Russian Chemical Bulletin</i> , 2020, 69, 1321-1328. | 0.4 | 6 |
| 13744 | Synthesis of Ultrasmall and Monodisperse Selenium-Doped Carbon Dots from Amino Acids for Free Radical Scavenging. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 16876-16883. | 1.8 | 13 |
| 13745 | MgC₆H₂ Isomers: Potential Candidates for Laboratory and Radioastronomical Studies. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7518-7525. | 1.1 | 10 |
| 13746 | Introductory lecture: when the density of the noninteracting reference system is not the density of the physical system in density functional theory. <i>Faraday Discussions</i> , 2020, 224, 9-26. | 1.6 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13747 | Extension of the Simmons–Smith reaction to metal-carbynes: efficient synthesis of metallacyclopropenes with π -aromaticity. <i>Chemical Science</i> , 2020, 11, 10159-10166. | 3.7 | 19 |
| 13748 | A novel anthracene derivative with an asymmetric structure as an electron transport material for stable Rec. 2020 blue organic light-emitting diodes. <i>Journal of Information Display</i> , 2020, 21, 197-201. | 2.1 | 5 |
| 13749 | Surface-Directed Disparity in Self-Assembled Structures of Small-Peptide α -Glutathione on Gold and Silver Nanoparticles. <i>Langmuir</i> , 2020, 36, 11255-11261. | 1.6 | 20 |
| 13750 | Bouncing off walls – widths of exit channels from shallow minima can dominate selectivity control. <i>Chemical Science</i> , 2020, 11, 9937-9944. | 3.7 | 17 |
| 13751 | Triangulenium dyes: the comprehensive photo-absorption and emission story of a versatile family of chromophores. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20673-20684. | 1.3 | 5 |
| 13752 | Gold-Catalyzed Cycloisomerization of 1,6-Cyclohexenylalkyne: An Efficient Entry to Bicyclo[3.2.1]oct-2-ene and Bicyclo[3.3.1]nonadiene. <i>Journal of Organic Chemistry</i> , 2020, 85, 12657-12669. | 1.7 | 15 |
| 13753 | Methoxy-substituted bis-tridentate iridium(III) phosphors and fabrication of blue organic light emitting diodes. <i>Journal of Materials Chemistry C</i> , 2020, 8, 13590-13602. | 2.7 | 14 |
| 13754 | Quantum-chemistry-aided ligand engineering for potential molecular switches: changing barriers to tune excited state lifetimes. <i>Chemical Communications</i> , 2020, 56, 11831-11834. | 2.2 | 4 |
| 13755 | A Highly Selective Perylenediimide-Based Chemosensor: “Naked-Eye” Colorimetric and Fluorescent Turn-On Recognition for Al^{3+} . <i>Frontiers in Chemistry</i> , 2020, 8, 702. | 1.8 | 9 |
| 13756 | Mechanistic Insights Into the Anticancer Properties of the Auranofin Analog $\text{Au}(\text{PET}_3)$: A Theoretical and Experimental Study. <i>Frontiers in Chemistry</i> , 2020, 8, 812. | 1.8 | 31 |
| 13757 | Mechanism for the reactivation of the peroxidase activity of human cyclooxygenases: investigation using phenol as a reducing cosubstrate. <i>Scientific Reports</i> , 2020, 10, 15187. | 1.6 | 5 |
| 13758 | Homo- and hetero-dinuclear $\text{Pt}(\text{II})/\text{Pd}(\text{II})$ complexes: studies of hydrolysis, nucleophilic substitution reactions, DNA/BSA interactions, DFT calculations, molecular docking and cytotoxic activity. <i>Dalton Transactions</i> , 2020, 49, 14411-14431. | 1.6 | 17 |
| 13759 | Bimetallic Bis-NHC-Ir(III) Complex Bearing 2-Arylbenzo[d]oxazolyl Ligand: Synthesis, Catalysis, and Bimetallic Effects. <i>Organometallics</i> , 2020, 39, 3514-3523. | 1.1 | 23 |
| 13760 | Antenna triplet DFT calculations to drive the design of luminescent Ln^{3+} complexes. <i>Dalton Transactions</i> , 2020, 49, 14556-14563. | 1.6 | 7 |
| 13761 | Alloying with Sn Suppresses Sintering of Size-Selected Subnano Pt Clusters on SiO_2 with and without Adsorbates. <i>Chemistry of Materials</i> , 2020, 32, 8595-8605. | 3.2 | 19 |
| 13762 | Shining light on the electronic structure and relaxation dynamics of the isolated oxyluciferin anion. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19022-19032. | 1.3 | 5 |
| 13763 | Establishing the accuracy of density functional approaches for the description of noncovalent interactions in biomolecules. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 21685-21695. | 1.3 | 4 |
| 13764 | Theoretical investigation on the nature of 4-substituted Hantzsch esters as alkylation agents. <i>RSC Advances</i> , 2020, 10, 31425-31434. | 1.7 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13765 | Chiral Molecules as Sensitive Probes for Direct Detection of $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"} \langle \text{mml:mi} \text{mathvariant="script"} \rangle \text{P} \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$ -Odd Cosmic Fields. <i>Physical Review Letters</i> , 2020, 125, 123004. | 2.9 | 15 |
| 13766 | Molecular structure, electronic properties and drug-likeness of xylazine by quantum methods and qsar analysis. <i>SN Applied Sciences</i> , 2020, 2, 1. | 1.5 | 2 |
| 13767 | Oxygen Atom Transfer Reactivity of Molybdenum(VI) Complexes Employing Pyrimidine- and Pyridine-2-thiolate Ligands. <i>Inorganic Chemistry</i> , 2020, 59, 14577-14593. | 1.9 | 17 |
| 13768 | Accessing distributions of exchange and dipolar couplings in stiff molecular rulers with Cu($\langle \text{scp} \rangle \text{ii} \langle \text{scp} \rangle$) centres. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 21707-21730. | 1.3 | 9 |
| 13769 | Breaking the axiality of pentagonalâ€“bipyramidal dysprosium($\langle \text{scp} \rangle \text{iii} \langle \text{scp} \rangle$) single-molecule magnets with pyrazolate ligands. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 4367-4376. | 3.0 | 7 |
| 13770 | Probing the conformational landscape and thermochemistry of DNA dinucleotide anions $\langle i \rangle \text{via} \langle /i \rangle$ helium nanodroplet infrared action spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 18400-18413. | 1.3 | 23 |
| 13771 | Photoinduced charge transfer in quasi-one-dimensional polymers in two-photon absorption. <i>RSC Advances</i> , 2020, 10, 33288-33298. | 1.7 | 3 |
| 13772 | How Big is the Pinacol Boronic Ester as a Substituent?. <i>Angewandte Chemie</i> , 2020, 132, 22589-22593. | 1.6 | 7 |
| 13773 | Structural characterization of supramolecular hollow nanotubes with atomistic simulations and SAXS. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 21083-21093. | 1.3 | 14 |
| 13774 | Accurate Hybrid Density Functionals with UW12 Correlation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6176-6194. | 2.3 | 5 |
| 13775 | A DFT Protocol for the Prediction of $\langle \text{sup} \rangle 31 \langle \text{sup} \rangle$ P NMR Chemical Shifts of Phosphine Ligands in First-Row Transition-Metal Complexes. <i>Organometallics</i> , 2020, 39, 3121-3130. | 1.1 | 15 |
| 13776 | Vibrational Dynamics of a Chiral Smectic Liquid Crystal Undergoing Vitrification and Cold Crystallization. <i>Crystals</i> , 2020, 10, 655. | 1.0 | 17 |
| 13777 | Molecular electrostatic potential at nuclear position as a new concept in evaluation of the substitution effects of intramolecular B/N frustrated Lewis pairs in H ₂ splitting and CO ₂ reduction. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26416. | 1.0 | 7 |
| 13778 | Green Approach for Visible-Light-Induced Direct Functionalization of 2-Methylquinolines. <i>Journal of Organic Chemistry</i> , 2020, 85, 11663-11678. | 1.7 | 4 |
| 13779 | Proton-Sensitive Free-Radical Dimer Evolution Is a Critical Control Point for the Synthesis of $\hat{\text{I}} \langle \text{sup} \rangle 2,2 \langle \text{sup} \rangle \hat{\text{I}} \langle \text{sup} \rangle$ -Bibenzothiazines. <i>Journal of Organic Chemistry</i> , 2020, 85, 11440-11448. | 1.7 | 5 |
| 13780 | Open-shell donorâ€“acceptor conjugated metal-free dyes for dye-sensitized solar cells. <i>Molecular Systems Design and Engineering</i> , 2020, 5, 1477-1490. | 1.7 | 9 |
| 13781 | Deriving the vibronic coupling constants of the cyclopentadienyl radical with density functional theory and GOWO. <i>Journal of Chemical Physics</i> , 2020, 153, 064303. | 1.2 | 2 |
| 13782 | Development and Investigation of an Organocatalytic Enantioselective [10 + 2] Cycloaddition. <i>ACS Catalysis</i> , 2020, 10, 10784-10793. | 5.5 | 23 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13783 | Assessing the Tammâ€“Dancoff approximation, singletâ€“singlet, and singletâ€“triplet excitations with the latest long-range corrected double-hybrid density functionals. <i>Journal of Chemical Physics</i> , 2020, 153, 064106. | 1.2 | 54 |
| 13785 | Polycyclic Aromatic Hydrocarbons and Dust Particle Surface Interactions: Catalytic Hydrogenation of Polycyclic Aromatic Hydrocarbon Molecules under Vacuum Conditions. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 1730-1742. | 1.2 | 5 |
| 13786 | Adaptive π -Aromaticity in an Unsaturated Threeâ€“Membered Ring. <i>Chemistry - an Asian Journal</i> , 2020, 15, 3444-3450. | 1.7 | 17 |
| 13787 | Synthesis and Thermochromic Luminescence of Ag(I) Complexes Based on 4,6-Bis(diphenylphosphino)-Pyrimidine. <i>Inorganics</i> , 2020, 8, 46. | 1.2 | 11 |
| 13788 | How Big is the Pinacol Boronic Ester as a Substituent?. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 22403-22407. | 7.2 | 32 |
| 13789 | Heteroatom-Rich Porous Carbons Derived from Nontoxic Green Organic Crystals for High-Performance Symmetric and Asymmetric Supercapacitors with Aqueous/Gel Electrolyte. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 13634-13647. | 3.2 | 13 |
| 13790 | Functionalized pyridine in pycen-based iron($\langle scp \rangle iii \langle /scp \rangle$) complexes: evaluation of fundamental properties. <i>RSC Advances</i> , 2020, 10, 31165-31170. | 1.7 | 9 |
| 13791 | Identification of decomposition reactions for HMDSO organosilicon using quantum chemical calculations. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26415. | 1.0 | 5 |
| 13792 | Rigorous Computational Study Reveals What Docking Overlooks: Double Trouble from Membrane Association in Protein Kinase C Modulators. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5624-5633. | 2.5 | 6 |
| 13793 | Rapid Detection of Strong Correlation with Machine Learning for Transition-Metal Complex High-Throughput Screening. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8067-8076. | 2.1 | 40 |
| 13794 | Parity-nonconserving interactions of electrons in chiral molecules with cosmic fields. <i>Physical Review A</i> , 2020, 102, . | 1.0 | 4 |
| 13795 | An Insight into the Excitation States of Small Molecular Semiconductor Y6. <i>Molecules</i> , 2020, 25, 4118. | 1.7 | 23 |
| 13796 | Magnetic Circular Dichroism of <i>meso</i> -Phenyl-Substituted Pd-Octaethylporphyrins. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8144-8158. | 1.1 | 6 |
| 13797 | Density Functional Theory Predictions of Noncovalent Hydrogen Isotope Effects during Octane Sorption to a Kaolinite Surface. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 1756-1764. | 1.2 | 1 |
| 13798 | 4,4â€“2,5,5â€“2-Tetraamino-3,3â€“2-azo-bis-1,2,4-triazole and the electrosynthesis of high-performing insensitive energetic materials. <i>Journal of Materials Chemistry A</i> , 2020, 8, 19337-19347. | 5.2 | 43 |
| 13799 | Harvesting of surface plasmon polaritons: Role of the confinement factor. <i>Journal of Chemical Physics</i> , 2020, 153, 094107. | 1.2 | 1 |
| 13800 | Scrutinizing â€œLigand Bandsâ€“via Polarized Single-Crystal X-ray Absorption Spectra of Copper(I) and Copper(II) Bis-2,2â€“bipyridine Species. <i>Inorganic Chemistry</i> , 2020, 59, 13416-13426. | 1.9 | 5 |
| 13801 | Multireaction Approach to Quantum Thermochemistry. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8088-8099. | 1.1 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13802 | A mixed-valence diruthenium(ii,iii) complex endowed with high stability: from experimental evidence to theoretical interpretation. <i>Dalton Transactions</i> , 2020, 49, 14520-14527. | 1.6 | 25 |
| 13803 | Catalytic Regioselective Benzoylation of 1,2- <i>trans</i> -Diols in Carbohydrates with Benzoyl Cyanide: The Axial Oxy Group Effect and the Action of Achiral and Chiral Amine Catalysts. <i>ACS Catalysis</i> , 2020, 10, 11406-11416. | 5.5 | 12 |
| 13804 | Deep-blue organic light-emitting diodes based on a doublet $d\text{f}$ transition cerium(III) complex with 100% exciton utilization efficiency. <i>Light: Science and Applications</i> , 2020, 9, 157. | 7.7 | 43 |
| 13805 | Probing the binding modes and dynamics of histidine on fumed silica surfaces by solid-state NMR. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20349-20361. | 1.3 | 12 |
| 13806 | A data-driven approach to determine dipole moments of diatomic molecules. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 24191-24200. | 1.3 | 11 |
| 13807 | A theoretical study of the reactivity of ethene and benzophenone with a hyper-coordinated alkene containing a so-called E=E (E = C, Si, Ge, Sn, and Pb) unit. <i>Dalton Transactions</i> , 2020, 49, 12842-12853. | 1.6 | 6 |
| 13808 | Versatility of the bis(iminopyrrolylmethyl)amine ligand: tautomerism, protonation, helical chirality, and the secondary coordination sphere with halogen bonds in the formation of copper(II) and nickel(II) complexes. <i>Dalton Transactions</i> , 2020, 49, 13840-13853. | 1.6 | 13 |
| 13809 | Lewis Acid-Base Interactions between Polysulfides and Boehmite Enables Stable Room-Temperature Sodium-Sulfur Batteries. <i>Advanced Functional Materials</i> , 2020, 30, 2005669. | 7.8 | 40 |
| 13810 | Mechanochemically Activated Asymmetric Organocatalytic Domino Mannich Reaction-Fluorination. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 14417-14424. | 3.2 | 28 |
| 13811 | Exploring the mechanism and counterion activity regulation in the Co^{III} (salen)-catalyzed hydration of propylene oxide. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22417-22425. | 1.3 | 5 |
| 13812 | A comprehensive study: Theoretical and experimental investigation of heteroatom and substituent effects on frontier orbitals and polymer solar cell performances. <i>Journal of Polymer Science</i> , 2020, 58, 2792-2806. | 2.0 | 11 |
| 13813 | Substituent Pattern Effects on the Redox Potentials of Quinone-Based Active Materials for Aqueous Redox Flow Batteries. <i>ChemSusChem</i> , 2020, 13, 5480-5488. | 3.6 | 33 |
| 13814 | Probing structural properties and antioxidant activity mechanisms for eleocarpanthraquinone. <i>Journal of Molecular Modeling</i> , 2020, 26, 233. | 0.8 | 29 |
| 13815 | Crystalline Molecular Standards for Low-Frequency Vibrational Spectroscopies. <i>Journal of Infrared, Millimeter, and Terahertz Waves</i> , 2020, 41, 1284-1300. | 1.2 | 9 |
| 13816 | On-the-Fly <i>ab initio</i> Semiclassical Evaluation of Electronic Coherences in Polyatomic Molecules Reveals a Simple Mechanism of Decoherence. <i>Physical Review Letters</i> , 2020, 125, 083001. | 2.9 | 21 |
| 13817 | Fullerene Thermochemical Stability: Accurate Heats of Formation for Small Fullerenes, the Importance of Structural Deformation on Reactivity, and the Special Stability of C_{60} . <i>Journal of Physical Chemistry A</i> , 2020, 124, 6688-6698. | 1.1 | 19 |
| 13818 | Energy landscape study of water splitting and H_2 evolution at a ruthenium(II) pincer complex. <i>Journal of Computational Chemistry</i> , 2020, 41, 2240-2250. | 1.5 | 1 |
| 13819 | Chiral tetranuclear copper(II) complexes: synthesis, optical and magnetic properties. <i>New Journal of Chemistry</i> , 2020, 44, 16845-16855. | 1.4 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13820 | Low pressure gas electron diffraction: An experimental setup and case studies. <i>Review of Scientific Instruments</i> , 2020, 91, 074104. | 0.6 | 2 |
| 13821 | A Natural Alkaloid, \hat{I}^2 -Carboline, as a One- and Two-Photon Responsive Fluorescent Photoremovable Protecting Group: Sequential Release of the Same or Different Carboxylic Acids. <i>Organic Letters</i> , 2020, 22, 6998-7002. | 2.4 | 13 |
| 13822 | Spectral shift, electronic coupling and exciton delocalization in nanocrystal dimers: insights from all-atom electronic structure computations. <i>Nanoscale</i> , 2020, 12, 18124-18136. | 2.8 | 6 |
| 13823 | Effect of substituents and promoters on the Diels-Alder cycloaddition reaction in the biorenewable synthesis of trimellitic acid. <i>RSC Advances</i> , 2020, 10, 30656-30670. | 1.7 | 11 |
| 13824 | Design and synthesis of organic dyes with various donor groups: promising dyes for dye-sensitized solar cells. <i>Bulletin of Materials Science</i> , 2020, 43, 1. | 0.8 | 3 |
| 13825 | Tailoring desolvation kinetics enables stable zinc metal anodes. <i>Journal of Materials Chemistry A</i> , 2020, 8, 19367-19374. | 5.2 | 136 |
| 13826 | First-principles investigation of band offset and charge transfer characteristics at the PE/fluorinated layer interface. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22207-22216. | 1.3 | 4 |
| 13827 | Computation of Dipole Moments: A Recommendation on the Choice of the Basis Set and the Level of Theory. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7538-7548. | 1.1 | 25 |
| 13828 | <i>In Silico</i> Investigation of Electronic Structure, Binding Patterns and Molecular Docking of Nevirapine: An anti-HIV Type-1 Drug. <i>Polycyclic Aromatic Compounds</i> , 2022, 42, 2789-2804. | 1.4 | 10 |
| 13829 | Evaluations of nonlocal electron-phonon couplings in tetracene, rubrene, and C10 \hat{a} ~DNBDT \hat{a} ~NW based on density functional theory. <i>Physical Review B</i> , 2020, 102, . | 1.1 | 11 |
| 13830 | Rapid Sequentially Palladium Catalyzed Four-Component Synthesis of Novel Fluorescent Biaryl-Substituted Isoxazoles. <i>Catalysts</i> , 2020, 10, 1412. | 1.6 | 5 |
| 13831 | Theoretical Investigations on the Excited-State Dynamics of an Al ³⁺ Fluorescence Sensor. <i>Journal of Physical Chemistry A</i> , 2020, 124, 11093-11101. | 1.1 | 7 |
| 13832 | Carbonyl Stretch as a Franck-Condon Active Mode and Driving Force for Excited-State Decay of 8-Methoxy-4-methyl-2H-benzo[<i>g</i>]chromen-2-one from $n\hat{I}^*$ State. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11472-11480. | 1.2 | 19 |
| 13833 | Mean-field density matrix decompositions. <i>Journal of Chemical Physics</i> , 2020, 153, 214109. | 1.2 | 10 |
| 13834 | Solvated State of Ethylenediamine in Nonaqueous Solvents, According to Quantum Chemical Data. <i>Russian Journal of Physical Chemistry A</i> , 2020, 94, 2051-2054. | 0.1 | 0 |
| 13835 | Comparison of computational chemistry methods for the discovery of quinone-based electroactive compounds for energy storage. <i>Scientific Reports</i> , 2020, 10, 22149. | 1.6 | 26 |
| 13836 | Theoretical Prediction on the New Types of Noble Gas Containing Anions OBONgO \hat{a} ~' and OCNNgO \hat{a} ~' (Ng=He, Ar, Kr and Xe). <i>Molecules</i> , 2020, 25, 5839. | 1.7 | 3 |
| 13837 | The role of high-order electron correlation effects in a model system for non-valence correlation-bound anions. <i>Journal of Chemical Physics</i> , 2020, 153, 224118. | 1.2 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13838 | On the Borate-Catalyzed Electrochemical Reduction of Phosphine Oxide: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10239-10245. | 1.1 | 4 |
| 13839 | DUAL EMISSION OF 2-AMINO-4-METHYLPYRIMIDINE: A THEORETICAL STUDY. <i>Journal of Structural Chemistry</i> , 2020, 61, 1521-1529. | 0.3 | 3 |
| 13840 | DFT and TD-DFT Study of Favipiravir Tautomerism as RNA Polymerase Inhibitors : COVID-19. <i>IOP Conference Series: Materials Science and Engineering</i> , 2020, 928, 072066. | 0.3 | 5 |
| 13841 | Pure Rotational Spectrum of Benzophenone Detected by Broadband Microwave Spectrometer in the 2â€“8 GHz Range. <i>Applied Sciences (Switzerland)</i> , 2020, 10, 8471. | 1.3 | 1 |
| 13842 | Why Conventional Design Rules for Câ€“H Activation Fail for Open-Shell Transition-Metal Catalysts. <i>ACS Catalysis</i> , 2020, 10, 15033-15047. | 5.5 | 30 |
| 13843 | Oxidation of Silver Cyanide $\text{Ag}(\text{CN})_2$ by the OH Radical: From <i>Ab Initio</i> Calculation to Molecular Simulation and to Experiment. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10787-10798. | 1.1 | 2 |
| 13844 | Unspecified verticality of Franck-Condon transitions, absorption and emission spectra of cyanine dyes, and a classically inspired approximation. <i>RSC Advances</i> , 2020, 10, 43153-43167. | 1.7 | 12 |
| 13845 | Emission redshift in DCM2-doped $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \langle \text{mml:m} \text{mathvariant="normal"} \text{Alq} \rangle \langle \text{mml:m} \text{mn} \rangle \langle \text{mml:m} \text{sub} \rangle \langle \text{mml:math} \rangle$ caused by nonlinear Stark shifts and FÃ¶rster-mediated exciton diffusion. <i>Physical Review B</i> , 2020, 102, . | 1.1 | 11 |
| 13846 | Electric-Field-Induced Effects on the Dipole Moment and Vibrational Modes of the Centrosymmetric Indigo Molecule. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10856-10869. | 1.1 | 18 |
| 13847 | Fluorophore-Appendant 5,5â€“Bicalixarene Scaffolds for Host-Guest Sensing of Nitric Oxide. <i>Organic Letters</i> , 2020, 22, 9706-9711. | 2.4 | 4 |
| 13848 | Stop Four Gaps with One Bush: Versatile Hierarchical Polybenzimidazole Nanoporous Membrane for Highly Durable Liâ€“S Battery. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 55809-55819. | 4.0 | 14 |
| 13849 | Physicochemical Properties of Choline Chloride-Based Deep Eutectic Solvents with Polyols: An Experimental and Theoretical Investigation. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 18712-18728. | 3.2 | 44 |
| 13850 | 1,2,3-Triazole substituted phthalocyanine metal complexes as potential inhibitors for anticholinesterase and antidiabetic enzymes with molecular docking studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 4429-4439. | 2.0 | 24 |
| 13851 | First-Principle Studies of Istradefylline with Emphasis on the Stability, Reactivity, Interactions and Wavefunction-Dependent Properties. <i>Polycyclic Aromatic Compounds</i> , 2020, , 1-15. | 1.4 | 15 |
| 13852 | Glucuronidation of Methylated Quercetin Derivatives: Chemical and Biochemical Approaches. <i>Journal of Agricultural and Food Chemistry</i> , 2020, 68, 14790-14807. | 2.4 | 9 |
| 13853 | Spectroscopic/Bond Property Relationship in Group 11 Dihydrides via Relativistic Four-Component Methods. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10565-10579. | 1.1 | 3 |
| 13854 | Pure rotational spectrum of dibenzofuran in range of 2âˆ“6â€“...GHz. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 125-128. | 0.6 | 1 |
| 13855 | Gas-phase spectroscopic characterization of neutral and ionic polycyclic aromatic phosphorus heterocycles (PAPHs). <i>Monthly Notices of the Royal Astronomical Society</i> , 2020, 500, 2564-2576. | 1.6 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13856 | Identification and Reactivity of <i>cis</i> , <i>cis</i> -Dihydroxycarbene, a New [CH ₂ O ₂] Intermediate. Journal of the American Chemical Society, 2020, 142, 19457-19461. | 6.6 | 5 |
| 13857 | Vibrationally resolved valence and core photoionization and photoexcitation spectra of an electron-deficient trivalent boron compound: the case of catecholborane. Physical Chemistry Chemical Physics, 2020, 22, 25396-25407. | 1.3 | 5 |
| 13858 | Atomistic origins of charge traps in CdSe nanoclusters. Physical Chemistry Chemical Physics, 2020, 22, 26299-26305. | 1.3 | 8 |
| 13859 | Microsolvation of myrtenal studied by microwave spectroscopy highlights the role of quasi-hydrogen bonds in the stabilization of its hydrates. Journal of Chemical Physics, 2020, 153, 104304. | 1.2 | 12 |
| 13860 | Rotational Spectroscopy Meets Quantum Chemistry for Analyzing Substituent Effects on Non-Covalent Interactions: The Case of the Trifluoroacetophenone-Water Complex. Molecules, 2020, 25, 4899. | 1.7 | 8 |
| 13861 | One-Pot Synthesis of ¹³ C-Pyrones from Aromatic Ketones/Heteroarenes and Carboxylic Acids. Journal of Organic Chemistry, 2020, 85, 15051-15061. | 1.7 | 4 |
| 13862 | Quantitative calculations of the non-radiative rate of phosphorescent Ir(III) complexes. Physical Chemistry Chemical Physics, 2020, 22, 27348-27356. | 1.3 | 9 |
| 13863 | Rational design of [2+2]-fusion induced high-performance DHP/CPD based photoswitches. Physical Chemistry Chemical Physics, 2020, 22, 26255-26264. | 1.3 | 2 |
| 13864 | New Directions in the Modeling of Organometallic Reactions. Topics in Organometallic Chemistry, 2020, , . | 0.7 | 1 |
| 13865 | Shedding Light on the Free Radical Nature of Sulfonated Melanins. Journal of Physical Chemistry B, 2020, 124, 10365-10373. | 1.2 | 18 |
| 13866 | Theoretical equilibrium shape of hydroxyapatite, revised. CrystEngComm, 2020, 22, 7944-7951. | 1.3 | 1 |
| 13867 | RCOSMO-CAMPD: Enhancing Reactions by Integrated Computer-Aided Design of Solvents and Processes based on Quantum Chemistry. Chemie-Ingenieur-Technik, 2020, 92, 1489-1500. | 0.4 | 9 |
| 13868 | Hybrid Boron-Carbon Chemistry. Molecules, 2020, 25, 5026. | 1.7 | 5 |
| 13869 | In Silico Modeling of Spirolides and Gymnodimines: Determination of S Configuration at Butenolide Ring Carbon C-4. Toxins, 2020, 12, 685. | 1.5 | 1 |
| 13870 | Acetylated cashew-gum-based silver nanoparticles for the development of latent fingerprints on porous surfaces. Environmental Nanotechnology, Monitoring and Management, 2020, 14, 100383. | 1.7 | 1 |
| 13871 | Origin of Selectivity in Protein Hydrolysis by Zr(IV)-Containing Metal Oxides as Artificial Proteases. ACS Catalysis, 2020, 10, 13455-13467. | 5.5 | 13 |
| 13872 | Computational refinement of the puzzling red tetrasulfur chromophore in ultramarine pigments. Physical Chemistry Chemical Physics, 2020, 22, 22684-22698. | 1.3 | 9 |
| 13873 | Development of gold(III) thiosemicarbazone complex-loaded PLGA nanoparticles: characterization and sustained release studies. Journal of Nanoparticle Research, 2020, 22, 1. | 0.8 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13874 | Comparative Study of the Biphasic Behavior of Cyanex301 and Its Two Analogs by Molecular Dynamics Simulations. <i>Advanced Theory and Simulations</i> , 2020, 3, 1900242. | 1.3 | 1 |
| 13875 | Magnetically Induced Alignment of Natural Products for Stereochemical Structure Determination via NMR. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15860-15864. | 7.2 | 11 |
| 13876 | Hybrid functional calculations of electro-optical properties of novel Ga _{1-x} In _x Te ternary chalcogenides. <i>Applied Physics A: Materials Science and Processing</i> , 2020, 126, 1. | 1.1 | 8 |
| 13877 | Synthesis, physical characterization, thermal studies, biological activities and DFT computations on the molecular structure and vibrational spectra of [C ₇ H ₁₂ N ₂] ₂ Bi ₂ Br ₁₀ ·4H ₂ O compound. <i>Journal of Solid State Chemistry</i> , 2020, 288, 121402. | 1.4 | 3 |
| 13878 | The low-barrier methyl internal rotation in the rotational spectrum of 3-methylphenylacetylene. <i>Journal of Molecular Structure</i> , 2020, 1213, 128109. | 1.8 | 6 |
| 13879 | Electronic and structural relations between solid CaB ₆ and the molecular dianion B ₆ H ₆ (²⁻): A computational study. <i>Solid State Sciences</i> , 2020, 102, 106169. | 1.5 | 0 |
| 13880 | Steric Effect Determines the Formation of Lactam Lactam Dimers or Amide C=O···NH (Lactam) Chain Motifs in <i>N</i> -Phenyl-2-hydroxynicotinanilides. <i>Crystal Growth and Design</i> , 2020, 20, 4346-4357. | 1.4 | 5 |
| 13881 | The one-electron self-interaction error in 74 density functional approximations: a case study on hydrogenic mono- and dinuclear systems. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15805-15830. | 1.3 | 27 |
| 13882 | The Lysosomotropic Activity of Hydrophobic Weak Base Drugs is Mediated via Their Intercalation into the Lysosomal Membrane. <i>Cells</i> , 2020, 9, 1082. | 1.8 | 32 |
| 13883 | A Theoretical Study of the Adsorption Process of B-aflatoxins Using <i>Pyracantha koidzumii</i> (Hayata) Rehder Biomasses. <i>Toxins</i> , 2020, 12, 283. | 1.5 | 7 |
| 13884 | How Do Local Reactivity Descriptors Shape the Potential Energy Surface Associated with Chemical Reactions? The Valence Bond Delocalization Perspective. <i>Journal of the American Chemical Society</i> , 2020, 142, 10102-10113. | 6.6 | 31 |
| 13885 | Solvent Organization and Rate Regulation of a Menshutkin Reaction by Oriented External Electric Fields are Revealed by Combined MD and QM/MM Calculations. <i>Journal of the American Chemical Society</i> , 2020, 142, 9955-9965. | 6.6 | 55 |
| 13886 | The role of the excited state dynamic of the antenna ligand in the lanthanide sensitization mechanism. <i>Dalton Transactions</i> , 2020, 49, 7444-7450. | 1.6 | 25 |
| 13887 | Synthesis and Characterization of Poly(hydrogen halide) Halogenates (H ₂ X). <i>Chemistry - A European Journal</i> , 2020, 26, 13256-13263. | 1.7 | 3 |
| 13888 | PSIXAS: A Psi4 plugin for efficient simulations of X-ray absorption spectra based on the transition potential and Kohn-Sham method. <i>Journal of Computational Chemistry</i> , 2020, 41, 1781-1789. | 1.5 | 21 |
| 13889 | Exploring the influence of water molecules on the stability of the cinnabar oxides. <i>Chemical Physics Letters</i> , 2020, 747, 137351. | 1.2 | 2 |
| 13890 | Antioxidant and cytotoxic activity of isoindole compounds in breast cancer cells (MCF-7). <i>Journal of Molecular Structure</i> , 2020, 1217, 128366. | 1.8 | 0 |
| 13891 | Synthesis and molecular dynamic simulation of a novel single ion conducting gel polymer electrolyte for lithium-ion batteries. <i>Polymer</i> , 2020, 201, 122568. | 1.8 | 26 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13892 | An efficient hybrid scheme for time dependent density functional theory. <i>Journal of Chemical Physics</i> , 2020, 152, 184104. | 1.2 | 10 |
| 13893 | Theoretical study of rhodium(III)-catalyzed synthesis of benzoxepine and coumarin. <i>Journal of Molecular Modeling</i> , 2020, 26, 143. | 0.8 | 0 |
| 13894 | Dye-Anchoring Modes at the Dye- TiO_2 Interface of N3- and N749-Sensitized Solar Cells Revealed by Glancing-Angle Pair Distribution Function Analysis. <i>Journal of Physical Chemistry C</i> , 2020, 124, 11935-11945. | 1.5 | 20 |
| 13895 | Modeling the Reaction of Carboxylic Acids and Isonitriles in a Self-Assembled Capsule. <i>Chemistry - A European Journal</i> , 2020, 26, 10861-10870. | 1.7 | 5 |
| 13896 | Reliable reduction potentials of diaryliodonium cations and aryl radicals in acetonitrile from high-level ab initio computations. <i>Electrochimica Acta</i> , 2020, 351, 136404. | 2.6 | 14 |
| 13897 | Environmentally Friendly and Regioselective One-Pot Synthesis of Imines and Oxazolidines Serinol Derivatives and Their Use for Rubber Cross-Linking. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 9356-9366. | 3.2 | 9 |
| 13898 | Highly-excited state properties of cumulenone chlorides in the vacuum-ultraviolet. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11838-11849. | 1.3 | 5 |
| 13899 | Substituent-dependent generation of tricyclic frameworks by the rhodium-catalyzed cycloisomerization of homopropargyl allene-alkynes: a theoretical study. <i>Dalton Transactions</i> , 2020, 49, 7406-7419. | 1.6 | 1 |
| 13900 | Luminescent $\text{Zn}(\text{II})$ and $\text{Cd}(\text{II})$ complexes with chiral 2,2'-bipyridine ligands bearing natural monoterpene groups: synthesis, speciation in solution and photophysics. <i>Dalton Transactions</i> , 2020, 49, 7552-7563. | 1.6 | 13 |
| 13901 | A bioinspired molybdenum-copper molecular catalyst for CO_2 electroreduction. <i>Chemical Science</i> , 2020, 11, 5503-5510. | 3.7 | 40 |
| 13902 | The $\text{Pd}(0)$ and $\text{Pd}(\text{II})$ cocatalyzed isomerization of alkynyl epoxides to furans: a mechanistic investigation using DFT calculations. <i>Dalton Transactions</i> , 2020, 49, 9223-9230. | 1.6 | 2 |
| 13903 | The ONETEP linear-scaling density functional theory program. <i>Journal of Chemical Physics</i> , 2020, 152, 174111. | 1.2 | 94 |
| 13904 | Double addition of phenylacetylene onto the mixed bridge phosphinito-phosphanido $\text{Pt}(\text{I})$ complex $[(\text{PhCy})_2\text{Pt}(\text{P}(\text{O})\text{Cy})_2]\text{Pt}(\text{P}(\text{O})\text{Cy})_2\text{Pt}(\text{P}(\text{O})\text{Cy})_2]$. <i>Dalton Transactions</i> , 2020, 49, 6776-6789. | 1.6 | 16 |
| 13905 | Mechanism and origins of stereo- and enantioselectivities of palladium-catalyzed hydroamination of racemic internal allenes via dynamic kinetic resolution: a computational study. <i>Organic Chemistry Frontiers</i> , 2020, 7, 1502-1511. | 2.3 | 21 |
| 13906 | Structural studies of 3-tert-butyl-8-(methylchalcogenyl)pyrazolo[5,1-c][1,2,4]triazin-4(1H)-ones. <i>Structural Chemistry</i> , 2020, 31, 1457-1470. | 1.0 | 11 |
| 13907 | Photoinduced Reactivity in a Dispiro-1,2,4-trioxolane: Adamantane Ring Expansion and First Direct Observation of the Long-Lived Triplet Diradical Intermediates. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4202-4210. | 1.1 | 7 |
| 13908 | Theoretical free energy profile and benchmarking of functionals for amino-thiourea organocatalyzed nitro-Michael addition reaction. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11529-11536. | 1.3 | 20 |
| 13909 | Mechanism of Catalysis by Asparaginase. <i>Biochemistry</i> , 2020, 59, 1927-1945. | 1.2 | 36 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 13910 | Solvent Mediated Excited State Proton Transfer in Indigo Carmine. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4156-4162. | 2.1 | 26 |
| 13911 | An open quantum system theory for polarizable continuum models. <i>Journal of Chemical Physics</i> , 2020, 152, 174114. | 1.2 | 14 |
| 13912 | Stereoselective [4+2]â€Cycloaddition with Chiral Alkenylboranes. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 11432-11439. | 7.2 | 16 |
| 13913 | Tuning Physicochemical Properties of Antipsychotic Drug Aripiprazole with Multicomponent Crystal Strategy Based on Structure and Property Relationship. <i>Crystal Growth and Design</i> , 2020, 20, 3747-3761. | 1.4 | 34 |
| 13914 | Completing density functional theory by machine learning hidden messages from molecules. <i>Npj Computational Materials</i> , 2020, 6, . | 3.5 | 121 |
| 13915 | Side-chain tuning in conjugated polymer photocatalysts for improved hydrogen production from water. <i>Energy and Environmental Science</i> , 2020, 13, 1843-1855. | 15.6 | 92 |
| 13916 | Stereoselective [4+2]â€Cycloaddition with Chiral Alkenylboranes. <i>Angewandte Chemie</i> , 2020, 132, 11529-11536. | 1.6 | 7 |
| 13917 | Organic Amines as Targeting Stabilizer at the Polymer/Fullerene Interface for Polymer:PC 61 BM Solar Cells. <i>Energy Technology</i> , 2020, 8, 2000266. | 1.8 | 8 |
| 13918 | Decoding chemical information from vibrational spectroscopy data: Local vibrational mode theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1480. | 6.2 | 85 |
| 13919 | Mechanism of antioxidant properties of quercetin and quercetin-DNA complex. <i>Journal of Molecular Modeling</i> , 2020, 26, 133. | 0.8 | 53 |
| 13920 | Electron Spin Densities and Density Functional Approximations: Open-Shell Polycyclic Aromatic Hydrocarbons as Case Study. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3567-3577. | 2.3 | 20 |
| 13921 | Renewable Aromatics from Tree-Borne Oils over Zeolite Catalysts Promoted by Transition Metals. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 24756-24766. | 4.0 | 21 |
| 13922 | Deconvolution of conformational exchange from Raman spectra of aqueous RNA nucleosides. <i>Communications Chemistry</i> , 2020, 3, . | 2.0 | 7 |
| 13923 | Outer-sphere effects on ligand-field excited-state dynamics: solvent dependence of high-spin to low-spin conversion in [Fe(bpy)3]2+. <i>Chemical Science</i> , 2020, 11, 5191-5204. | 3.7 | 11 |
| 13924 | ReSpect: Relativistic spectroscopy DFT program package. <i>Journal of Chemical Physics</i> , 2020, 152, 184101. | 1.2 | 90 |
| 13925 | Development of nearâ€infrared firefly luciferin analogue reacted with wildâ€type and mutant luciferases. <i>Chirality</i> , 2020, 32, 922-931. | 1.3 | 14 |
| 13926 | Sensitive Energetics from the <i>N</i>-Amination of 4â€Nitroâ€1,2,3â€Triazole. <i>ChemistryOpen</i> , 2020, 9, 806-819. | 1.9 | 11 |
| 13927 | Î²-Carboline copper complex as a potential mitochondrial-targeted anticancer chemotherapeutic agent: Favorable attenuation of human breast cancer MCF7 cells via apoptosis. <i>Saudi Journal of Biological Sciences</i> , 2020, 27, 2164-2173. | 1.8 | 11 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 13928 | Theoretical Insights into the Excited State Decays of a Donor–Acceptor Dyad: Is the Twisted and Rehybridized Intramolecular Charge-Transfer State Involved?. <i>Journal of Physical Chemistry B</i> , 2020, 124, 4564-4572. | 1.2 | 20 |
| 13929 | Arene–Ruthenium(II) Complexes Containing 11 <i>H</i> -Indeno[1,2- <i>b</i>]quinoxalin-11-one Derivatives and Tryptanthrin-6-oxime: Synthesis, Characterization, Cytotoxicity, and Catalytic Transfer Hydrogenation of Aryl Ketones. <i>ACS Omega</i> , 2020, 5, 11167-11179. | 1.6 | 20 |
| 13930 | FB-REDA: fragment-based decomposition analysis of the reorganization energy for organic semiconductors. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11881-11890. | 1.3 | 10 |
| 13931 | Borohydride catalyzed redistribution reaction of hydrosilane and chlorosilane: a potential system for facile preparation of hydrochlorosilanes. <i>RSC Advances</i> , 2020, 10, 17404-17407. | 1.7 | 2 |
| 13932 | Synthesis of anti-4-phenoxyphenylaminoglyoxime and its some transition metal complexes: Spectral, DFT, electrochemical and anticancer activity studies. <i>Journal of Molecular Structure</i> , 2020, 1215, 128190. | 1.8 | 3 |
| 13933 | Evaluation of conformational and spectral behavior and prediction of biological activity and chemical reactivity descriptors of Levosimendan. <i>Journal of Molecular Structure</i> , 2020, 1217, 128464. | 1.8 | 0 |
| 13934 | Catalytic hydration of cyanamides with phosphinous acid-based ruthenium(II) and osmium(II) complexes: scope and mechanistic insights. <i>Catalysis Science and Technology</i> , 2020, 10, 4084-4098. | 2.1 | 9 |
| 13935 | Thermally induced intra-molecular transformation and metalation of free-base porphyrin on Au(111) surface steered by surface confinement and ad-atoms. <i>Nanoscale Advances</i> , 2020, 2, 2986-2991. | 2.2 | 8 |
| 13936 | Formation of bis-benzimidazole and bis-benzoxazole through organocatalytic depolymerization of poly(ethylene terephthalate) and its mechanism. <i>Polymer Chemistry</i> , 2020, 11, 4904-4913. | 1.9 | 13 |
| 13937 | Levels and inhalation health risk of neonicotinoid insecticides in fine particulate matter (PM _{2.5}) in urban and rural areas of China. <i>Environment International</i> , 2020, 142, 105822. | 4.8 | 46 |
| 13938 | Density Functional Theory investigation of rhombohedral multiferroic oxides for photocatalytic water splitting and organic photodegradation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 400, 112656. | 2.0 | 16 |
| 13939 | Heterobimetallic η^2 -carbido complexes of platinum and tungsten. <i>Dalton Transactions</i> , 2020, 49, 8143-8161. | 1.6 | 12 |
| 13940 | Synthesis, characterization and photoinduced CO-release by manganese(II) complexes. <i>New Journal of Chemistry</i> , 2020, 44, 10892-10901. | 1.4 | 9 |
| 13941 | Theoretical and Experimental Investigations of Large Stokes Shift Fluorophores Based on a Quinoline Scaffold. <i>Molecules</i> , 2020, 25, 2488. | 1.7 | 28 |
| 13942 | Hydrogen/deuterium adsorption and absorption properties on and in palladium using a combined plane wave and localized basis set method. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26275. | 1.0 | 4 |
| 13943 | Theoretical study and antimicrobial activities of New Schiff base derivatives with thiophene. <i>Journal of Molecular Structure</i> , 2020, 1218, 128522. | 1.8 | 15 |
| 13944 | O-Phosphination of Aldehydes/Ketones toward Phosphoric Esters: Experimental and Mechanistic Studies. <i>Organic Letters</i> , 2020, 22, 4742-4748. | 2.4 | 28 |
| 13945 | Exploring the Reaction Mechanism of H_2S Decomposition with MS_3 ($M = Mo,$) Tj ETQq1 1.0.784314 rgBT / Ov | 1.6 | 14 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 13946 | Modulation of the photoelectrochemical behavior of Au nanocluster@TiO ₂ electrode by doping. <i>Chemical Science</i> , 2020, 11, 6248-6255. | 3.7 | 20 |
| 13947 | Synergism of anisotropic and computational NMR methods reveals the likely configuration of phormidolide A. <i>Chemical Communications</i> , 2020, 56, 7565-7568. | 2.2 | 20 |
| 13948 | A Close Look at the Molecular Structure, Prototropic Behavior and Supramolecular Architecture of (E)-4-Bromo-2-[(phenylimino)methyl]-5-methoxyphenol by Spectroscopic, Crystallographic, and Computational Methods. <i>Crystallography Reports</i> , 2020, 65, 457-462. | 0.1 | 1 |
| 13949 | Investigation of the Molecular Structure of (E)-2-Bromo-6-[(4-bromo-2-methylphenylimino)methyl]-4-chlorophenol. <i>Crystallography Reports</i> , 2020, 65, 463-467. | 0.1 | 2 |
| 13950 | Non-symmetrical Sterically Challenged Phenanthroline Ligands and Their Homoleptic Copper(I) Complexes with Improved Excited-State Properties. <i>Chemistry - A European Journal</i> , 2020, 26, 11887-11899. | 1.7 | 19 |
| 13951 | Nucleophilic Substitution Reaction of Pentafluorophenyl Aminated Perylene Diimide system with N,N-Dimethylformamide. <i>Asian Journal of Organic Chemistry</i> , 2020, 9, 1076-1080. | 1.3 | 3 |
| 13952 | Highly Sensitive Real-Time Isotopic Quantification of Water by ATR-FTIR. <i>Analytical Chemistry</i> , 2020, 92, 7500-7507. | 3.2 | 2 |
| 13953 | Ab initio study of parity and time-reversal violation in laser-coolable triatomic molecules. <i>Physical Review A</i> , 2020, 101, . | 1.0 | 31 |
| 13954 | Quantum chemical mass spectrometry: Ab initio study of b ² ion formation mechanisms for the singly protonated Gln-His-Ser tripeptide. <i>Rapid Communications in Mass Spectrometry</i> , 2020, 34, e8778. | 0.7 | 4 |
| 13955 | An sp-hybridized all-carboatomic ring, cyclo[18]carbon: Bonding character, electron delocalization, and aromaticity. <i>Carbon</i> , 2020, 165, 468-475. | 5.4 | 188 |
| 13956 | Synthesis, crystal structure and magnetic properties of tetranuclear copper complex based on [(4-bromophenyl)(hydroxy)methylene]bis(phosphonic acid). <i>Inorganica Chimica Acta</i> , 2020, 509, 119689. | 1.2 | 2 |
| 13957 | Anion Photoelectron Spectroscopy and Theoretical Study of H _{Au} CN and [H _{Au} CN] ⁻ : Spin-Orbit Coupling and Low-Lying Excited States. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4712-4719. | 1.1 | 1 |
| 13958 | Thermodynamics of high-temperature aluminum, zirconium, and yttrium hydroxide and oxyhydroxide vapor species. <i>Journal of the American Ceramic Society</i> , 2020, 103, 5870-5880. | 1.9 | 4 |
| 13959 | Mechanism Study of Molecular Deformation of 2,2',5',2''-Tetramethylated p-Terphenyl-4,4''-dithiol Trapped in Gold Junctions. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4456-4461. | 2.1 | 5 |
| 13960 | Spin-chemical effects on intramolecular photoinduced charge transfer reactions in bisphenanthroline copper(viologen)-viologen dyad assemblies. <i>Chemical Science</i> , 2020, 11, 5511-5525. | 3.7 | 0 |
| 13961 | A General Hypoxia-Responsive Molecular Container for Tumor-Targeted Therapy. <i>Advanced Materials</i> , 2020, 32, e1908435. | 11.1 | 81 |
| 13962 | Der Einfluss von Aggregation auf die Photophysik von spiroverbrückten Heterotriangulenen. <i>Angewandte Chemie</i> , 2020, 132, 16368-16376. | 1.6 | 6 |
| 13963 | Oxidation, Coordination, and Nickel-Mediated Deconstruction of a Highly Electron-Rich Diboron Analogue of 1,3,5-Hexatriene. <i>Angewandte Chemie</i> , 2020, 132, 15847-15855. | 1.6 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13964 | Biologically-Active Heterocyclic Molecules with Aggregation-Induced Blue-Shifted Emission and Efficient Luminescence both in Solution and Solid States. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 400, 112642. | 2.0 | 18 |
| 13965 | Experimental and theoretical studies on monoazo dye including diphenylamine and N-methyldiphenylamine derivatives. <i>Journal of Molecular Structure</i> , 2020, 1217, 128449. | 1.8 | 3 |
| 13966 | A dual attack on the peroxide bond. The common principle of peroxidatic cysteine or selenocysteine residues. <i>Redox Biology</i> , 2020, 34, 101540. | 3.9 | 24 |
| 13967 | Vibrational mode frequency correction of liquid water in density functional theory molecular dynamics simulations with van der Waals correction. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12785-12793. | 1.3 | 9 |
| 13968 | Enhancing Magnetic Hysteresis in Single-Molecule Magnets by Ligand Functionalization. <i>CheM</i> , 2020, 6, 1777-1793. | 5.8 | 103 |
| 13969 | Removing organic harmful compounds from the polluted water by a novel synthesized cobalt(II) and titanium(IV) containing photocatalyst under visible light. <i>Environmental Nanotechnology, Monitoring and Management</i> , 2020, 14, 100304. | 1.7 | 3 |
| 13970 | Bond Dissociation Energy of Peroxides Revisited. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4742-4751. | 1.1 | 37 |
| 13971 | Achieving Site-Selectivity for C-H Activation Processes Based on Distance and Geometry: A Carpenter's Approach. <i>Journal of the American Chemical Society</i> , 2020, 142, 10571-10591. | 6.6 | 236 |
| 13972 | Exact Generalized Kohn-Sham Theory for Hybrid Functionals. <i>Physical Review X</i> , 2020, 10, . | 2.8 | 19 |
| 13973 | Diboran(4)azide als stabile Quelle für kurzlebige Iminborane. <i>Angewandte Chemie</i> , 2020, 132, 15608-15614. | 1.6 | 7 |
| 13974 | The Impact of Aggregation on the Photophysics of Spiro-Bridged Heterotriangulenes. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 16233-16240. | 7.2 | 10 |
| 13975 | Triquinoline-versus Fullerene-Based Cycloparaphenylene Ionic Complexes: Comparison of Photoinduced Charge-Shift Reactions. <i>Chemistry - A European Journal</i> , 2020, 26, 10896-10902. | 1.7 | 10 |
| 13976 | Theoretical investigation of the molecular structure, vibrational spectra, thermodynamic and nonlinear optical properties of 4, 5-dibromo-2, 7-dinitro- fluorescein. <i>Optical and Quantum Electronics</i> , 2020, 52, 1. | 1.5 | 12 |
| 13977 | First-principles study on the structure and optical spectroscopy of the redox-active center of blue copper proteins. <i>Chemical Physics</i> , 2020, 537, 110859. | 0.9 | 1 |
| 13978 | Isomeric Differentiation and Acidic Metabolite Identification by Piperidine-Based Tagging, LC-MS/MS, and Understanding of the Dissociation Chemistries. <i>Analytical Chemistry</i> , 2020, 92, 9305-9311. | 3.2 | 5 |
| 13979 | XO-PBC: An Accurate and Efficient Method for Molecular Crystals. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4271-4285. | 2.3 | 10 |
| 13980 | Relationships between Orbital Energies, Optical and Fundamental Gaps, and Exciton Shifts in Approximate Density Functional Theory and Quasiparticle Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4337-4350. | 2.3 | 21 |
| 13981 | Quantum Mechanical Modeling of Reaction Rate Acceleration in Microdroplets. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4984-4989. | 1.1 | 33 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 13982 | Hole Transfer in Cumulenenic and Polyynic Carbynes. <i>Journal of Physical Chemistry C</i> , 2020, 124, 12834-12849. | 1.5 | 4 |
| 13983 | Spin Splitting Energy of Transition Metals: A New, More Affordable Wave Function Benchmark Method and Its Use to Test Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4416-4428. | 2.3 | 38 |
| 13984 | Decomposition pathway and kinetic analysis of perfluoroketone C ₅ F ₁₀ O. <i>Journal Physics D: Applied Physics</i> , 2020, 53, 415502. | 1.3 | 21 |
| 13985 | Assessing Cu ₂ L ₂ X ₄ dimeric moieties as ferromagnetic building blocks in double halide-bridged polymers (X = Cl ⁻ , Br ⁻ and L = benzamide). An experimental and computational study. <i>Polyhedron</i> , 2020, 185, 114603. | 1.0 | 2 |
| 13986 | Water stable molecular n-doping produces organic electrochemical transistors with high transconductance and record stability. <i>Nature Communications</i> , 2020, 11, 3004. | 5.8 | 82 |
| 13987 | Modification of a H-terminated silicon surface by organic sulfide molecules: the mechanism and origin of reactivity. <i>New Journal of Chemistry</i> , 2020, 44, 11056-11063. | 1.4 | 0 |
| 13988 | Oxidative Amidation of Amines in Tandem with Transamidation: A Route to Amides Using Visible-Light Energy. <i>Journal of Organic Chemistry</i> , 2020, 85, 9219-9229. | 1.7 | 28 |
| 13989 | Efficient Construction of Excited-State Hessian Matrices with Machine Learning Accelerated Multilayer Energy-Based Fragment Method. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5684-5695. | 1.1 | 27 |
| 13990 | Theoretical elucidation of the multi-functional synthetic methodology for switchable Ni(0)-catalyzed C-H allylations, alkenylations and dienylations with allenes. <i>Catalysis Science and Technology</i> , 2020, 10, 4219-4228. | 2.1 | 8 |
| 13991 | Charge density of 4-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]thiazole-2(3H)-thione. A comprehensive multipole refinement, maximum entropy method and density functional theory study. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2020, 76, 450-468. | 0.5 | 3 |
| 13992 | Adsorption studies on air pollutants using blue phosphorene nanosheet as a chemical sensor – DFT approach. <i>Computational and Theoretical Chemistry</i> , 2020, 1186, 112910. | 1.1 | 23 |
| 13993 | Vibrational spectrum of 1-ethyl-3-methylimidazolium tetrafluoroborate on graphene surface. <i>Journal of Molecular Liquids</i> , 2020, 311, 113340. | 2.3 | 5 |
| 13994 | Data-Driven Approaches Can Overcome the Cost–Accuracy Trade-Off in Multireference Diagnostics. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4373-4387. | 2.3 | 28 |
| 13995 | Assessment of the DLPNO Binding Energies of Strongly Noncovalent Bonded Atmospheric Molecular Clusters. <i>ACS Omega</i> , 2020, 5, 7601-7612. | 1.6 | 38 |
| 13996 | Intermacrocyclic Interactions upon Stepwise Oxidations in a Monometallic Porphyrin Dimer: Ring versus Metal–Center Oxidations and Effect of Counter Anions. <i>Chemistry - A European Journal</i> , 2020, 26, 14405-14418. | 1.7 | 5 |
| 13997 | Photoelectron spectra and electronic structure of boron diacetate formazanates. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 238, 118441. | 2.0 | 4 |
| 13998 | Incorporating Electronic Information into Machine Learning Potential Energy Surfaces via Approaching the Ground-State Electronic Energy as a Function of Atom-Based Electronic Populations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4256-4270. | 2.3 | 50 |
| 13999 | Space Charge-Limited Current Transport Mechanism in Crossbar Junction Embedding Molecular Spin Crossovers. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 31696-31705. | 4.0 | 15 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14000 | Effect of spin-phonon interactions on Urbach tails in flexible [M ₂ (bdc) ₂ (dabco)]. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15242-15247. | 1.3 | 8 |
| 14001 | Energy Level Engineering in Organic Thin Films by Tailored Halogenation. <i>Advanced Functional Materials</i> , 2020, 30, 2002987. | 7.8 | 9 |
| 14002 | Effect of chitosan/albendazole nanocarriers™ solvation by molecular dynamics. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1. | 0.5 | 5 |
| 14003 | The aromatic fullerene-like silicon cage with 12 Si ₅ pentagons stabilized by a V ₃ unit. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1. | 0.5 | 6 |
| 14004 | Impact of Quantum Chemistry Parameter Choices and Cluster Distribution Model Settings on Modeled Atmospheric Particle Formation Rates. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5931-5943. | 1.1 | 34 |
| 14005 | Uncovering Alternate Pathways to Nafion Membrane Degradation in Fuel Cells with First-Principles Modeling. <i>Journal of Physical Chemistry C</i> , 2020, 124, 15094-15106. | 1.5 | 6 |
| 14006 | Synthesis of Cyclometalated Platinum(II) Complex with an Alkynyl-Substituted Isocyanide Ligand, Its Structure and Photophysical Properties. <i>Russian Journal of General Chemistry</i> , 2020, 90, 648-654. | 0.3 | 6 |
| 14007 | Magneto-optical coupling and Kerr effect in PbNiO ₃ , PbCrO ₃ , and PbMnO ₃ multiferroics: An excited-states approach. <i>Journal of Magnetism and Magnetic Materials</i> , 2020, 514, 167176. | 1.0 | 7 |
| 14008 | Interpolative Separable Density Fitting Decomposition for Accelerating Hartree-Fock Exchange Calculations within Numerical Atomic Orbitals. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5664-5674. | 1.1 | 18 |
| 14009 | DFT benchmark study of the O-O bond dissociation energy in peroxides validated with high-level ab initio calculations. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1. | 0.5 | 6 |
| 14010 | Molecular anchoring stabilizes low valence Ni(<i>scpt</i>)TPP on copper against thermally induced chemical changes. <i>Journal of Materials Chemistry C</i> , 2020, 8, 8876-8886. | 2.7 | 13 |
| 14011 | Enamine Barbiturates and Thiobarbiturates as a New Class of Bacterial Urease Inhibitors. <i>Applied Sciences (Switzerland)</i> , 2020, 10, 3523. | 1.3 | 5 |
| 14012 | Magnetically Induced Alignment of Natural Products for Stereochemical Structure Determination via NMR. <i>Angewandte Chemie</i> , 2020, 132, 15994-15998. | 1.6 | 1 |
| 14013 | Visible Light-Driven Dehydrogenation of Benzylamine under Liberation of H ₂ . <i>ChemCatChem</i> , 2020, 12, 4593-4599. | 1.8 | 10 |
| 14014 | Self-assembly of multifunctional hydrogels with polyoxometalates helical arrays using nematic peptide liquid crystal template. <i>Journal of Colloid and Interface Science</i> , 2020, 578, 218-228. | 5.0 | 16 |
| 14015 | Distinct Roles of Ag(I) and Cu(II) as Cocatalysts in Achieving Positional-Selective C-H Alkenylation of Isoxazoles: A Theoretical Investigation. <i>Journal of Organic Chemistry</i> , 2020, 85, 8387-8396. | 1.7 | 9 |
| 14016 | The "Dark Side" of Germanium-Based Photoinitiators™ Connecting Redox Properties and Optical Absorption. <i>Organometallics</i> , 2020, 39, 2257-2268. | 1.1 | 3 |
| 14017 | Computational study of catalyst-controlled regiodivergent pathways in hydroboration of 1,3-dienes: mechanism and origin of regioselectivity. <i>Organic Chemistry Frontiers</i> , 2020, 7, 2157-2167. | 2.3 | 11 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14018 | Novel non-spherical deltahedra in tetramolybdaborane structures: Generation of low-energy structures by capping Mo ₄ B ₄ cubes. <i>Polyhedron</i> , 2020, 187, 114626. | 1.0 | 1 |
| 14019 | Investigations on crystal structure of a novel 3-((4,6-dimethylpyrimidin-2-yl)amino)isobenzofuran-1(3H)-one, and related theoretical studies. <i>Arabian Journal of Chemistry</i> , 2020, 13, 5564-5580. | 2.3 | 8 |
| 14020 | Investigation of structural, spectral, electronic, and biological properties of 1,3-disubstituted benzimidazole derivatives. <i>Journal of Molecular Structure</i> , 2020, 1219, 128582. | 1.8 | 18 |
| 14021 | Synthesis, Photophysics, and Reverse Saturable Absorption of <i>trans</i> -Bis-cyclometalated Iridium(III) Complexes (C ^{N^C})Ir(R-tpy) (tpy = 2,2',6',6'-Terpyridine) with Broadband Excited-State Absorption. <i>Inorganic Chemistry</i> , 2020, 59, 8532-8542. | 1.9 | 14 |
| 14022 | Assembly of Thiosubstituted Benzoxazoles via Copper-Catalyzed Coupling of Thiols with 5-Iodotriazoles Serving as Diazo Surrogates. <i>Journal of Organic Chemistry</i> , 2020, 85, 9015-9028. | 1.7 | 15 |
| 14023 | Real-time detection of single-molecule reaction by plasmon-enhanced spectroscopy. <i>Science Advances</i> , 2020, 6, eaba6012. | 4.7 | 41 |
| 14024 | Molecular Interpretation of Pharmaceuticals™ Adsorption on Carbon Nanomaterials: Theory Meets Experiments. <i>Processes</i> , 2020, 8, 642. | 1.3 | 29 |
| 14025 | Magnesium and Nickel Cyclacenes with Dewar and Ladenburg Defects. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5408-5414. | 1.1 | 10 |
| 14026 | One electron reduction transforms high-valent low-spin cobalt alkylidene into high-spin cobalt(II) carbene radical. <i>Chemical Communications</i> , 2020, 56, 8416-8419. | 2.2 | 8 |
| 14027 | Mechanisms and origin of regioselectivity on N-heterocyclic carbene-catalyzed [3+2]/[4+2] annulations of C ₆₀ with α,β -unsaturated aldehydes. <i>Molecular Catalysis</i> , 2020, 493, 111045. | 1.0 | 3 |
| 14028 | On the radicalar properties of graphene fragments: double-hybrid DFT and perturbation theory approaches. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1. | 0.5 | 1 |
| 14029 | Sodium and lithium one-dimensional coordination polymers with 1H-indazole-3-carboxylic acid: Crystal structures, vibrational spectra and DFT calculations. <i>Polyhedron</i> , 2020, 187, 114661. | 1.0 | 4 |
| 14030 | Mechano-Optical Switching of a Single Molecule with Doublet Emission. <i>ACS Nano</i> , 2020, 14, 8931-8938. | 7.3 | 11 |
| 14031 | Simulation of Thermophysical Properties of Phenylpropanolamine Drug in Water by Ab Initio and DFT Methods. <i>Russian Journal of Physical Chemistry A</i> , 2020, 94, 1173-1179. | 0.1 | 0 |
| 14032 | Synthese eines gegenanionstabilisierten Bis(silylium)ions. <i>Angewandte Chemie</i> , 2020, 132, 10609-10613. | 1.6 | 5 |
| 14033 | Mechanistic Investigation into the Acetate-Initiated Catalytic Trimerization of Aliphatic Isocyanates: A Bicyclic Ride. <i>Journal of Organic Chemistry</i> , 2020, 85, 8553-8562. | 1.7 | 8 |
| 14034 | Investigation of Ferrocene Linkers in β -Substituted Porphyrins. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5513-5522. | 1.1 | 6 |
| 14035 | Consecutive and Extensive Transition of Luminescent Color of an Organic Solid Material by Applying High Pressure. <i>Journal of Physical Chemistry C</i> , 2020, 124, 14911-14917. | 1.5 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14036 | Experimental and quantum chemical study of the DNA/protein binding and the biological activity of a rhodium(III) complex with 1,2,4-triazole as an inert ligand. Dalton Transactions, 2020, 49, 9070-9085. | 1.6 | 19 |
| 14037 | Effect of substituents in sulfoxides on the enhancement of thermoelectric properties of PEDOT:PSS: experimental and modelling evidence. Molecular Systems Design and Engineering, 2020, 5, 976-984. | 1.7 | 29 |
| 14038 | Layered Crystal Structural Entecavir Monohydrate: Prepared in Pure Water and Calculated by DFT. Crystal Research and Technology, 2020, 55, 2000007. | 0.6 | 0 |
| 14039 | Parallel Implementation of Density Functional Theory Methods in the Quantum Interaction Computational Kernel Program. Journal of Chemical Theory and Computation, 2020, 16, 4315-4326. | 2.3 | 25 |
| 14040 | Triggered singlet fission via tuning current density vectors (CDV) in the ground-state and excited-state. Organic Electronics, 2020, 84, 105795. | 1.4 | 1 |
| 14041 | Hydrogen Migration-Triggered Diradicaloid Singlet-Fission Switch. Journal of the American Chemical Society, 2020, 142, 11791-11803. | 6.6 | 11 |
| 14042 | Structural, Spectroscopic, Electronic and Optical Properties of Novel Platinum Doped (PMMA/ZrO ₂) and (PMMA/Al ₂ O ₃) Nanocomposites for Electronics Devices. Transactions on Electrical and Electronic Materials, 2020, 21, 550-563. | 1.0 | 50 |
| 14043 | Near-infrared pH responsive heptamethine cyanine platforms: Modulating the proton acceptor. Dyes and Pigments, 2020, 181, 108611. | 2.0 | 15 |
| 14044 | Analyzing electron transfer properties of ferrocene in gasoline by cyclic voltammetry and theoretical methods. Microchemical Journal, 2020, 158, 105116. | 2.3 | 18 |
| 14045 | Experimental and theoretical investigations of the [Ln(2-dik)(NO ₃) ₂ (phen) ₂] \cdot nH ₂ O luminescent complexes. Journal of Luminescence, 2020, 226, 117455. | 1.5 | 13 |
| 14046 | Perylene derivative films: Emission from higher singlet excited state. Journal of Luminescence, 2020, 226, 117478. | 1.5 | 1 |
| 14047 | Formal synthesis of cochlearol A, a meroterpenoid with renoprotective activity. Tetrahedron Letters, 2020, 61, 151845. | 0.7 | 13 |
| 14048 | Tertiary Phosphine and Arsinic Complexes of Phosphorus Pentafluoride: Synthesis, Properties, and Electronic Structures. Inorganic Chemistry, 2020, 59, 4517-4526. | 1.9 | 3 |
| 14049 | Competing ultrafast photoinduced electron transfer and intersystem crossing of [Re(CO) ₃ (Dmp)(His124)(Trp122)] ⁺ in Pseudomonas aeruginosa azurin: a nonadiabatic dynamics study. Theoretical Chemistry Accounts, 2020, 139, 65. | 0.5 | 17 |
| 14050 | Unexpected hydrodefluorination of 3-Cl-tetrafluoropyridine. Interpretation through analysis of the potential energy surface for its radical anion. Journal of Fluorine Chemistry, 2020, 234, 109513. | 0.9 | 4 |
| 14051 | Effects of carboxylic acid auxiliary ligands on the magnetic properties of azido-Cu(II) complexes: A density functional theory study. Polyhedron, 2020, 182, 114506. | 1.0 | 14 |
| 14052 | Theoretical study on thermal curing mechanism of arylethynyl-containing resins. Physical Chemistry Chemical Physics, 2020, 22, 6468-6477. | 1.3 | 10 |
| 14053 | Accurate Quantum Chemical Calculation of Ionization Potentials: Validation of the DFT-LOC Approach via a Large Data Set Obtained from Experiments and Benchmark Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2020, 16, 2109-2123. | 2.3 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14054 | Hydrogen-Deuterium Exchange in Basic Near-Critical and Supercritical Media: An Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2530-2536. | 1.1 | 4 |
| 14055 | Prospects of Heterogeneous Hydroformylation with Supported Single Atom Catalysts. <i>Journal of the American Chemical Society</i> , 2020, 142, 5087-5096. | 6.6 | 98 |
| 14056 | Suppressing triplet decay in quinoidal singlet fission materials: the role of molecular planarity and rigidity. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7546-7551. | 1.3 | 4 |
| 14057 | An Overview of Self-Consistent Field Calculations Within Finite Basis Sets. <i>Molecules</i> , 2020, 25, 1218. | 1.7 | 37 |
| 14058 | Anti-fibrotic activity of gold and platinum complexes of Au(I) compounds as a new class of anti-fibrotic agents. <i>Journal of Inorganic Biochemistry</i> , 2020, 206, 111023. | 1.5 | 9 |
| 14059 | Evaluating Computational Shortcuts in Supercell-Based Phonon Calculations of Molecular Crystals: The Instructive Case of Naphthalene. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2716-2735. | 2.3 | 21 |
| 14060 | Quantitative assessment of the nature of noncovalent interactions in <i>N</i> -substituted-5-(adamantan-1-yl)-1,3,4-thiadiazole-2-amines: insights from crystallographic and QTAIM analysis. <i>RSC Advances</i> , 2020, 10, 9840-9853. | 1.7 | 28 |
| 14061 | ESIPT triggered TICT of an Al ³⁺ fluorescence sensor and its sensing mechanism. <i>Journal of Luminescence</i> , 2020, 223, 117203. | 1.5 | 8 |
| 14062 | Molecular generation targeting desired electronic properties via deep generative models. <i>Nanoscale</i> , 2020, 12, 6744-6758. | 2.8 | 27 |
| 14063 | Performance of TDDFT Vertical Excitation Energies of Core-Substituted Naphthalene Diimides. <i>Journal of Computational Chemistry</i> , 2020, 41, 1448-1455. | 1.5 | 21 |
| 14064 | New class of cocogem surfactants based on hexamethylenediamine, propylene oxide, and long chain carboxylic acids: Theory and application. <i>Journal of Industrial and Engineering Chemistry</i> , 2020, 86, 123-135. | 2.9 | 11 |
| 14065 | Triethanolamine lactate-supported nanomagnetic cellulose: a green and efficient catalyst for the synthesis of pyrazolo[3,4- <i>b</i>]quinolines and theoretical study. <i>Research on Chemical Intermediates</i> , 2020, 46, 2749-2765. | 1.3 | 19 |
| 14066 | Water enhanced mechanism for CO ₂ Methanol conversion. <i>Chemical Physics Letters</i> , 2020, 746, 137298. | 1.2 | 3 |
| 14067 | Acetaldehyde adsorption and detection: A density functional theory study on Al-doped graphene. <i>Vacuum</i> , 2020, 175, 109279. | 1.6 | 30 |
| 14068 | Bimetallic Ru-Mo Phosphide Catalysts for the Hydrogenation of CO ₂ to Methanol. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 6931-6943. | 1.8 | 24 |
| 14069 | The Role of the Hydrogen Bond between Piperazine and Fullerene Molecules in Stabilizing Polymer:Fullerene Solar Cell Performance. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 15472-15481. | 4.0 | 15 |
| 14070 | Experimental and DFT study of the effect of mercaptosuccinic acid on cyanide-free immersion gold deposition. <i>RSC Advances</i> , 2020, 10, 9768-9776. | 1.7 | 5 |
| 14071 | Structure-Property Relationships in Unsymmetric Bis(antiaromatics): Who Wins the Battle between Pentalene and Benzocyclobutadiene?. <i>Journal of Organic Chemistry</i> , 2020, 85, 5158-5172. | 1.7 | 19 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14072 | Unraveling the Lithium Bis(trifluoromethanesulfonyl)imide (LiTFSI) Doping Mechanism of Regioregular Poly(3-hexylthiophene): Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 7061-7070. | 1.5 | 14 |
| 14073 | Coking-Resistant Sub-Nano Dehydrogenation Catalysts: Pt _n Sn _x /SiO ₂ (<i>n</i> = 4, 7). <i>ACS Catalysis</i> , 2020, 10, 4543-4558. | 5.5 | 40 |
| 14074 | Visible-light-induced photocatalyst-free C-3 functionalization of indoles with diethyl bromomalonate. <i>Green Chemistry</i> , 2020, 22, 2543-2548. | 4.6 | 24 |
| 14075 | Extension and evaluation of the D4 London-dispersion model for periodic systems. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8499-8512. | 1.3 | 138 |
| 14076 | Probing the strong magnetic exchange behaviour of transition metal radical complexes: a DFT case study. <i>Dalton Transactions</i> , 2020, 49, 4539-4548. | 1.6 | 8 |
| 14077 | Predicting HSE band gaps from PBE charge densities via neural network functionals. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 155901. | 0.7 | 16 |
| 14078 | Biological evaluation of novel thiomaltol-based organometallic complexes as topoisomerase III± inhibitors. <i>Journal of Biological Inorganic Chemistry</i> , 2020, 25, 451-465. | 1.1 | 16 |
| 14079 | Alternating magnetic field mediated release of fluorophores from magnetic nanoparticles by hysteretic heating. <i>Journal of Colloid and Interface Science</i> , 2020, 571, 348-355. | 5.0 | 9 |
| 14080 | Photocatalytic proton reduction by a computationally identified, molecular hydrogen-bonded framework. <i>Journal of Materials Chemistry A</i> , 2020, 8, 7158-7170. | 5.2 | 45 |
| 14081 | Identifying Thermal Decomposition Products of Nitrate Ester Explosives Using Gas Chromatography–Vacuum Ultraviolet Spectroscopy: An Experimental and Computational Study. <i>Applied Spectroscopy</i> , 2020, 74, 1486-1495. | 1.2 | 10 |
| 14082 | Quantum Chemical Lipophilicities of Antimalarial Drugs in Relation to Terminal Half-Life. <i>ACS Omega</i> , 2020, 5, 6500-6515. | 1.6 | 1 |
| 14083 | Impurity Effects on Habit Change and Polymorphic Transitions in the System: Aragonite–Calcite–Vaterite. <i>Crystal Growth and Design</i> , 2020, 20, 2497-2507. | 1.4 | 11 |
| 14084 | Synthesis of a Counteranion-Stabilized Bis(silylium) Ion. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 10523-10526. | 7.2 | 16 |
| 14085 | Structural, optical, and surface morphological studies of ethyl cellulose/graphene oxide nanocomposites. <i>Polymer Composites</i> , 2020, 41, 2792-2802. | 2.3 | 85 |
| 14086 | Control of Ziegler–Natta catalyst activity by the structural design of alkoxy silane-based external donors. <i>New Journal of Chemistry</i> , 2020, 44, 6845-6852. | 1.4 | 11 |
| 14087 | Liquid-phase decomposition mechanism for bis(triaminoguanidinium) azotetrazolate (TAGzT). <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7314-7328. | 1.3 | 6 |
| 14088 | Theoretical Analysis of the Mechanism of the 1,3-Dipolar Cycloaddition of Benzodiazepine with N-Aryl-C-ethoxycarbonylnitrilimine. <i>Journal of Chemistry</i> , 2020, 2020, 1-8. | 0.9 | 2 |
| 14089 | Simple Trans-Platinum Complex Bearing 3-Aminoflavone Ligand Could Be a Useful Drug: Structure-Activity Relationship of Platinum Complex in Comparison with Cisplatin. <i>International Journal of Molecular Sciences</i> , 2020, 21, 2116. | 1.8 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14090 | Solid-State NMR Techniques for the Structural Characterization of Cyclic Aggregates Based on Borane-Phosphane Frustrated Lewis Pairs. <i>Molecules</i> , 2020, 25, 1400. | 1.7 | 10 |
| 14091 | Ruthenium(II)-Catalyzed Double Annulation of Quinones: Step-Economical Access to Valuable Bioactive Compounds. <i>Chemistry - A European Journal</i> , 2020, 26, 10981-10986. | 1.7 | 22 |
| 14092 | The Reaction of Sulfur Dioxide Radical Cation with Hydrogen and its Relevance in Solar Geoengineering Models. <i>ChemPhysChem</i> , 2020, 21, 1146-1156. | 1.0 | 7 |
| 14093 | Criegee intermediate decomposition pathways for the formation of o-toluic acid and 2-methylphenylformate. <i>Chemical Physics Letters</i> , 2020, 748, 137399. | 1.2 | 0 |
| 14094 | Dynamical properties of organo lead-halide perovskites and their interfaces to titania: insights from Density Functional Theory. <i>Heliyon</i> , 2020, 6, e03427. | 1.4 | 4 |
| 14095 | Natural transition orbitals for complex $\langle \text{SCP} \rangle$ excited state calculations. <i>Journal of Computational Chemistry</i> , 2020, 41, 1557-1563. | 1.5 | 15 |
| 14096 | Structures and vertical detachment energies of water cluster anions $(\text{H}_2\text{O})_n^-$ with $n = 11$. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1. | 0.5 | 4 |
| 14097 | NMR crystallography of molecular organics. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2020, 118-119, 10-53. | 3.9 | 95 |
| 14098 | Computational Study of Photocatalytic CO_2 Reduction by a Ni(II) Complex Bearing an S_2N_2 -Type Ligand. <i>Organometallics</i> , 2020, 39, 1176-1186. | 1.1 | 4 |
| 14099 | Free-base porphyrins with localized NH protons. Can substituents alone stabilize the elusive <i>cis</i> tautomer?. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 2861-2865. | 1.5 | 6 |
| 14100 | F-Centers in BaBrI Single Crystal. <i>IEEE Transactions on Nuclear Science</i> , 2020, 67, 946-951. | 1.2 | 4 |
| 14101 | High-Valent Metal-Oxo Species at the Nodes of Metal-Triazolate Frameworks: The Effects of Ligand Exchange and Two-State Reactivity for C-H Bond Activation. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 19494-19502. | 7.2 | 14 |
| 14102 | Describing Polytopal Rearrangements of Fluxional Molecules with Curvilinear Coordinates Derived from Normal Vibrational Modes: A Conceptual Extension of Cremer-Pople Puckering Coordinates. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3162-3193. | 2.3 | 8 |
| 14103 | Seeing Is Believing: Experimental Spin States from Machine Learning Model Structure Predictions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3286-3299. | 1.1 | 48 |
| 14104 | Curcumin analogs as the inhibitors of TLR4 pathway in inflammation and their drug like potentialities: a computer-based study. <i>Journal of Receptor and Signal Transduction Research</i> , 2020, 40, 324-338. | 1.3 | 19 |
| 14105 | Aromaticity and sterics control whether a cationic olefin radical is resistant to disproportionation. <i>Chemical Science</i> , 2020, 11, 4138-4149. | 3.7 | 29 |
| 14106 | <i>N</i> -Heterocyclic Silylenes as Ligands in Transition Metal Carbonyl Chemistry: Nature of Their Bonding and Supposed Innocence. <i>Chemistry - A European Journal</i> , 2020, 26, 11276-11292. | 1.7 | 27 |
| 14107 | From Neutral Aniline to Aniline Trication: A Computational and Experimental Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3120-3134. | 1.1 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 14108 | High-Valent Metal-Oxo Species at the Nodes of Metal-Triazolate Frameworks: The Effects of Ligand Exchange and Two-State Reactivity for C-H Bond Activation. <i>Angewandte Chemie</i> , 2020, 132, 19662-19670. | 1.6 | 9 |
| 14109 | Hydrogen evolution from water using heteroatom substituted fluorene conjugated co-polymers. <i>Journal of Materials Chemistry A</i> , 2020, 8, 8700-8705. | 5.2 | 47 |
| 14110 | Identification of Water Hexamer on Cu(111) Surfaces. <i>Journal of the American Chemical Society</i> , 2020, 142, 6902-6906. | 6.6 | 14 |
| 14111 | Transient proton transfer of base pair hydrogen bonds induced by intense terahertz radiation. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9316-9321. | 1.3 | 17 |
| 14112 | Structure, Spectral Properties, and Complexing Ability of 1-Phenyl-3-methylpyrazol-5-one Ferrocenoyl Hydrazone. <i>Russian Journal of General Chemistry</i> , 2020, 90, 257-267. | 0.3 | 1 |
| 14113 | Microcavity Enhanced Raman Spectroscopy of Fullerene C60 Bucky Balls. <i>Sensors</i> , 2020, 20, 1470. | 2.1 | 4 |
| 14114 | Heavy Atom Effect of Selenium for Metal-Free Phosphorescent Light-Emitting Diodes. <i>Chemistry of Materials</i> , 2020, 32, 2583-2592. | 3.2 | 86 |
| 14115 | Modified Clerodanes from the Essential Oil of <i>Dodonea viscosa</i> Leaves. <i>Molecules</i> , 2020, 25, 850. | 1.7 | 5 |
| 14116 | Tautomeric Equilibria of Nucleobases in the Hachimoji Expanded Genetic Alphabet. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2766-2777. | 2.3 | 22 |
| 14117 | Spectral Decomposition of the Reaction Force Constant. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2372-2379. | 1.1 | 6 |
| 14118 | Bidentate Schiff Base Ligands Appended Metal(II) Complexes as Probes of DNA and Plasma Protein: In Silico Molecular Modelling Studies. <i>Applied Biochemistry and Biotechnology</i> , 2020, 191, 1515-1532. | 1.4 | 14 |
| 14119 | Molecular Structure and Modeling of Water-Air and Ice-Air Interfaces Monitored by Sum-Frequency Generation. <i>Chemical Reviews</i> , 2020, 120, 3633-3667. | 23.0 | 97 |
| 14120 | Tailoring Hot Exciton Dynamics in 2D Hybrid Perovskites through Cation Modification. <i>ACS Nano</i> , 2020, 14, 3621-3629. | 7.3 | 38 |
| 14121 | Cobalt complexes of redox noninnocent azo-aromatic pincers. Isolation, characterization, and application as catalysts for the synthesis of quinazolin-4(3H)-ones. <i>Dalton Transactions</i> , 2020, 49, 8448-8459. | 1.6 | 22 |
| 14122 | The devil in the details: A tutorial review on some undervalued aspects of density functional theory calculations. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26332. | 1.0 | 63 |
| 14123 | Dealing with Spin States in Computational Organometallic Catalysis. <i>Topics in Organometallic Chemistry</i> , 2020, , 191-226. | 0.7 | 9 |
| 14124 | A search of a quantitative quantum-chemical approach for radiolytic stability prediction. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14992-14997. | 1.3 | 7 |
| 14125 | Probing the Electronic Structure of a Thorium Nitride Complex by Solid-State ¹⁵ N NMR Spectroscopy. <i>Inorganic Chemistry</i> , 2020, 59, 10138-10145. | 1.9 | 26 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14126 | Synthesis, Structures, and Antibacterial Activities of Four Similar 1D Metal-Organic Polymers with Different Metal Ions. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2020, 646, 532-539. | 0.6 | 4 |
| 14127 | Electronic effect of a perfluorinated \hat{I}^2 -diketiminato ligand on the bonding nature of copper carbonyl complexes. <i>Dalton Transactions</i> , 2020, 49, 9773-9780. | 1.6 | 9 |
| 14128 | In-plane polarization induced by the hydrogen bonding and π - π stacking of functionalized PDI supramolecules for the efficient photocatalytic degradation of organic pollutants. <i>Materials Chemistry Frontiers</i> , 2020, 4, 2673-2687. | 3.2 | 24 |
| 14129 | Anionic Copolymerization of Styrene Sulfide with Elemental Sulfur (S ₈). <i>Materials</i> , 2020, 13, 2597. | 1.3 | 21 |
| 14130 | Interaction and Reactivity of Cisplatin Physisorbed on Graphene Oxide Nano-Prototypes. <i>Nanomaterials</i> , 2020, 10, 1074. | 1.9 | 7 |
| 14131 | Evaluation of in vitro inhibitory effects of some natural compounds on tyrosinase activity and molecular docking study: Antimelanogenesis potential. <i>Journal of Biochemical and Molecular Toxicology</i> , 2020, 34, e22566. | 1.4 | 19 |
| 14132 | Substituted Ortho-Benzynes: Properties of the Triple Bond. <i>Journal of Organic Chemistry</i> , 2020, 85, 9905-9914. | 1.7 | 6 |
| 14133 | Computational mechanistic investigation of the Fe + CO ₂ \rightarrow FeO + CO reaction. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16943-16948. | 1.3 | 1 |
| 14134 | Range-separated hybrid and double-hybrid density functionals: A quest for the determination of the range-separation parameter. <i>Journal of Chemical Physics</i> , 2020, 152, 244124. | 1.2 | 24 |
| 14135 | Reaction Mechanism, Origins of Enantioselectivity, and Reactivity Trends in Asymmetric Allylic Alkylation: A Comprehensive Quantum Mechanics Investigation of a C(sp ³)-C(sp ³) Cross-Coupling. <i>Journal of the American Chemical Society</i> , 2020, 142, 13917-13933. | 6.6 | 37 |
| 14136 | Radiosynthesis, molecular modeling and biodistribution of ^{99m} Tc-Protoporphyrin as a preclinical model for tumor diagnosis. <i>Journal of Porphyrins and Phthalocyanines</i> , 2020, 24, 1174-1188. | 0.4 | 0 |
| 14137 | Structural and Optical Properties of Solvated PbI ₂ in \hat{I}^3 -Butyrolactone: Insight into the Solution Chemistry of Lead Halide Perovskite Precursors. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 6139-6145. | 2.1 | 15 |
| 14138 | Assessment of the Performance of Optimally Tuned Range-Separated Hybrid Functionals for Nuclear Magnetic Shielding Calculations. <i>Advanced Theory and Simulations</i> , 2020, 3, 2000083. | 1.3 | 7 |
| 14139 | Interactions of CO ₂ with cluster models of metal-organic frameworks. <i>Journal of Computational Chemistry</i> , 2020, 41, 2066-2083. | 1.5 | 0 |
| 14140 | DFT calculation and experimental study on electronic structure and optical properties of 7-Amino-4-oxo-3-(2-(2-thienyl)vinyl)-4H,8H-[1,2,4]triazino[3,4-b][1,3,4]thiadiazine-8-carbonitrile thin films. <i>Optik</i> , 2020, 220, 165199. | 1.4 | 10 |
| 14141 | Performance of DFT functionals for properties of small molecules containing beryllium, tungsten and hydrogen. <i>Nuclear Materials and Energy</i> , 2020, 22, 100731. | 0.6 | 8 |
| 14142 | Accurate high-resolution single-crystal diffraction data from a Pilatus3000 X CdTe detector. <i>Journal of Applied Crystallography</i> , 2020, 53, 635-649. | 1.9 | 28 |
| 14143 | Effect of the electronic state on low-rank coals with Ca ²⁺ ion exchange. <i>Journal of Molecular Structure</i> , 2020, 1218, 128544. | 1.8 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14144 | Difficulties of Popular Density Functionals to Describe the Conformational Isomerism in Iodoacetic Acid. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5570-5579. | 1.1 | 2 |
| 14145 | Exploring the Mechanism of Catalysis with the Unified Reaction Valley Approach (URVA) – A Review. <i>Catalysts</i> , 2020, 10, 691. | 1.6 | 20 |
| 14146 | Effect of 1,3-Propane Sultone on the Formation of Solid Electrolyte Interphase at Li-Ion Battery Anode Surface: A First-Principles Study. <i>ACS Omega</i> , 2020, 5, 13541-13547. | 1.6 | 9 |
| 14147 | Intermolecular Allene Functionalization by Silver-Nitrene Catalysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 13062-13071. | 6.6 | 25 |
| 14148 | Using electronegativity and hardness to test density functionals. <i>Journal of Chemical Physics</i> , 2020, 152, 244113. | 1.2 | 5 |
| 14149 | Alzheimer's disease: unraveling APOE4 binding to amyloid-beta peptide and lipids with molecular dynamics and quantum mechanics. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 5026-5032. | 2.0 | 3 |
| 14150 | The Structure of the "Vibration Hole" around an Isotopic Substitution – Implications for the Calculation of Nuclear Magnetic Resonance (NMR) Isotopic Shifts. <i>Molecules</i> , 2020, 25, 2915. | 1.7 | 3 |
| 14151 | Synthesis and Characterization of a 2,3-Dialkoxynaphthalene-Based Conjugated Copolymer via Direct Arylation Polymerization (DAP) for Organic Electronics. <i>Polymers</i> , 2020, 12, 1377. | 2.0 | 10 |
| 14152 | Calculating and Characterizing the Charge Distributions in Solids. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5884-5892. | 2.3 | 29 |
| 14153 | Applying support-vector machine learning algorithms toward predicting host-guest interactions with cucurbit[7]uril. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14976-14982. | 1.3 | 3 |
| 14154 | Rearrangement of 7-Aryloxazo[5,4- <i>b</i>]pyridines to Benzo[<i>c</i>][1,7]naphthyridine-4(3- <i>H</i>)-ones and Thieno[3,2- <i>c</i>][1,7]naphthyridine-6(7- <i>H</i>)-ones. <i>Journal of Organic Chemistry</i> , 2020, 85, 10072-10082. | 1.7 | 10 |
| 14155 | Gaining Insight into the Effect of Organic Interface Layer on Suppressing Ion Migration Induced Interfacial Degradation in Perovskite Solar Cells. <i>Advanced Functional Materials</i> , 2020, 30, 2000837. | 7.8 | 29 |
| 14156 | Quantum chemical topology at the spin-orbit configuration interaction level: Application to astatine compounds. <i>Journal of Computational Chemistry</i> , 2020, 41, 2055-2065. | 1.5 | 10 |
| 14157 | Structure and interaction properties of MBIL [Bmim][FeCl ₄] and methanol: A combined FTIR and simulation study. <i>Journal of Molecular Liquids</i> , 2020, 309, 113061. | 2.3 | 26 |
| 14158 | Reactions of Alkynes with Quasi-Linear 3d Metal(I) Silylamides of Chromium to Cobalt: A Comparative Study. <i>Inorganic Chemistry</i> , 2020, 59, 9521-9537. | 1.9 | 27 |
| 14159 | Mechanistic Insight into Bis(amino) Copper Formate Thermochemistry for Conductive Molecular Ink Design. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 33039-33049. | 4.0 | 14 |
| 14160 | β-Cyclodextrin Polymerized in Cross-Flowing Channels of Biomass Sawdust for Rapid and Highly Efficient Pharmaceutical Pollutants Removal from Water. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 32817-32826. | 4.0 | 28 |
| 14161 | Nickel-catalyzed hydroalkenylation of styrene with phenylpropanal: theoretical studies on the mechanism, regioselectivity, and role of phenylboronic acid. <i>Organic Chemistry Frontiers</i> , 2020, 7, 2207-2215. | 2.3 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14162 | Predicting the chemical reactivity of organic materials using a machine-learning approach. <i>Chemical Science</i> , 2020, 11, 7813-7822. | 3.7 | 32 |
| 14163 | Supramolecular Assemblies of Trinuclear Copper(II)-Pyrazolato Units: A Structural, Magnetic and EPR Study. <i>Chemistry</i> , 2020, 2, 626-644. | 0.9 | 4 |
| 14164 | Polymerizable Oxime Esters: An Efficient Photoinitiator with Low Migration Ability for 3D Printing to Fabricate Luminescent Devices. <i>ChemPhotoChem</i> , 2020, 4, 5296-5303. | 1.5 | 33 |
| 14165 | Competing excited-state deactivation processes in bacteriophytochromes. <i>Advances in Quantum Chemistry</i> , 2020, , 243-268. | 0.4 | 2 |
| 14166 | Theoretical kinetics of the $C_2H_4 + NH_2$ reaction. <i>Combustion and Flame</i> , 2020, 215, 193-202. | 2.8 | 5 |
| 14167 | Functionalization of N_2 via Formal 1,3-Haloboration of a Tungsten(0) π -Nitrogen Complex. <i>Chemistry - A European Journal</i> , 2020, 26, 16019-16027. | 1.7 | 12 |
| 14168 | Phosphorescent Cationic Heterodinuclear Ir^{III}/M^{I} Complexes ($M=Cu, Au$) with a Hybrid Janus-Type N -Heterocyclic Carbene Bridge. <i>Chemistry - A European Journal</i> , 2020, 26, 11751-11766. | 1.7 | 4 |
| 14169 | What is the nature of bonding in $[Fe(CO)_3(NO)]^+$ and $[Fe(CO)_4]_2^+$?. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1. | 0.5 | 4 |
| 14170 | MgC_2H_2 isomers – simple penta-atomic molecules missing in the laboratory. <i>Chemical Physics</i> , 2020, 538, 110899. | 0.9 | 10 |
| 14171 | Permanganyl chloride-mediated oxidation of tetramethylethylene: A density functional theory study. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 98, 107616. | 1.3 | 3 |
| 14172 | Diastereoselective Synthesis of P-Stereogenic Secondary Phosphine Oxides (SPOs) Bearing a Chiral Substituent by Ring Opening of (+)-Limonene Oxide with Primary Phosphido Nucleophiles. <i>Journal of Organic Chemistry</i> , 2020, 85, 14516-14526. | 1.7 | 8 |
| 14173 | Advances in the Molecular Catalysis of Dioxygen Reduction. <i>ACS Catalysis</i> , 2020, 10, 2640-2655. | 5.5 | 76 |
| 14174 | Is the origin of green fluorescence in unsymmetrical four-ring bent-core liquid crystals single or double proton transfer?. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4731-4740. | 1.3 | 11 |
| 14175 | Insights into plasmon induced keto-enol isomerization. <i>Nanoscale</i> , 2020, 12, 4334-4340. | 2.8 | 3 |
| 14176 | Predicting fluorescence quantum yields for molecules in solution: A critical assessment of the harmonic approximation and the choice of the lineshape function. <i>Journal of Chemical Physics</i> , 2020, 152, 054107. | 1.2 | 35 |
| 14177 | Group 13-15 Needle-Shaped Oligomers and Nanorods: Structures and Electronic Properties. , 2020, , 201-268. | | 1 |
| 14178 | Kinetics, mechanism and density functional theory calculations on base hydrolysis of β -amino acid esters catalyzed by $[Pd(AEMP)(H_2O)_2]^{2+}$ (AEMP = 2-(2-aminoethyl)-1-methylpyrrolidine). <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2020, 129, 613-626. | 0.8 | 0 |
| 14179 | The dynamic parallel distribution algorithm for hybrid density-functional calculations in HONPAS package. <i>Computer Physics Communications</i> , 2020, 254, 107204. | 3.0 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14180 | Spin Transition of an Iron(II) Organoborate Complex in Different Polymorphs and in Vacuum-Deposited Thin Films: Influence of Cooperativity. <i>Inorganic Chemistry</i> , 2020, 59, 7966-7979. | 1.9 | 24 |
| 14181 | H-Bonding on spin centres enhances spin-spin coupling for organic diradicals. <i>Journal of Materials Chemistry C</i> , 2020, 8, 3402-3408. | 2.7 | 8 |
| 14182 | In Silico Strategies in Tuberculosis Drug Discovery. <i>Molecules</i> , 2020, 25, 665. | 1.7 | 50 |
| 14183 | Oriented (Local) Electric Fields Drive the Millionfold Enhancement of the H-Abstraction Catalysis Observed for Synthetic Metalloenzyme Analogues. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 7915-7920. | 7.2 | 45 |
| 14184 | Nitro-imidazole-based ruthenium complexes with antioxidant and anti-inflammatory activities. <i>Journal of Inorganic Biochemistry</i> , 2020, 206, 111048. | 1.5 | 25 |
| 14185 | Stability Series for the Complexation of Six Key Siderophore Functional Groups with Uranyl Using Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2460-2472. | 1.1 | 11 |
| 14186 | Flame-retarding battery cathode materials based on reversible multi-electron redox chemistry of phenothiazine-based polymer. <i>Journal of Energy Chemistry</i> , 2020, 47, 256-262. | 7.1 | 17 |
| 14187 | The Impact of Macrocycle Conformation on the Taxadiene-Forming Carbocation Cascade: Insight Gained from Sobralene, a Recently Discovered Verticillene Isomer. <i>Journal of Organic Chemistry</i> , 2020, 85, 4507-4514. | 1.7 | 3 |
| 14188 | The Challenge of Reproducing with Calculations Raw Experimental Kinetic Data for an Organic Reaction. <i>Organic Letters</i> , 2020, 22, 2873-2877. | 2.4 | 25 |
| 14189 | Synthesis of New C-3 Substituted Kynurenic Acid Derivatives. <i>Molecules</i> , 2020, 25, 937. | 1.7 | 12 |
| 14190 | Charting Hydrogen Bond Anisotropy. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2846-2856. | 2.3 | 11 |
| 14191 | Iodization Threshold in Size-Dependent Reactions of Lead Clusters Pb _n ⁺ with Iodomethane. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2505-2512. | 1.1 | 5 |
| 14192 | Aminoalkyl radicals as halogen-atom transfer agents for activation of alkyl and aryl halides. <i>Science</i> , 2020, 367, 1021-1026. | 6.0 | 285 |
| 14193 | Synthesis and In Vitro Anticancer Evaluation of Novel Chrysin and 7-Aminochrysin Derivatives. <i>Molecules</i> , 2020, 25, 888. | 1.7 | 17 |
| 14194 | Synthesis, structural, spectroscopic, and thermal studies of some transition-metal complexes of a ligand containing the amino mercapto triazole moiety. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5591. | 1.7 | 28 |
| 14195 | Strategies for Design of Potential Singlet Fission Chromophores Utilizing a Combination of Ground-State and Excited-State Aromaticity Rules. <i>Journal of the American Chemical Society</i> , 2020, 142, 5602-5617. | 6.6 | 86 |
| 14196 | Correlating Solution- and Solid-State Structures of Conformationally Flexible Resorcinarenes: Significance of a Sulfonyl Group in Intramolecular Self-Inclusion. <i>Chemistry - A European Journal</i> , 2020, 26, 7374-7383. | 1.7 | 5 |
| 14197 | Asymptotic Behavior of the Exchange-Correlation Energy Density and the Kohn-Sham Potential in Density Functional Theory: Exact Results and Strategy for Approximations. <i>Israel Journal of Chemistry</i> , 2020, 60, 805-822. | 1.0 | 14 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 14198 | A Ditopic Phosphaneâ€‘decorated Benzenedithiol as Scaffold for Diâ€‘ and Trinuclear Complexes of Groupâ€‘10 Metals and Gold. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2020, 646, 769-776. | 0.6 | 1 |
| 14199 | Absorption spectra of xanthenes in aqueous solution: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5929-5941. | 1.3 | 23 |
| 14200 | QSAR studies on benzothiophene derivatives as Plasmodium falciparum Nâ€‘myristoyltransferase inhibitors: Molecular insights into affinity and selectivity. <i>Drug Development Research</i> , 2020, , . | 1.4 | 6 |
| 14201 | Quantum chemical predictions of waterâ€‘octanol partition coefficients applied to the SAMPL6 logP blind challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 485-493. | 1.3 | 13 |
| 14202 | Carbohydrate-Binding Capability and Functional Conformational Changes of AbnE, an Arabino-oligosaccharide Binding Protein. <i>Journal of Molecular Biology</i> , 2020, 432, 2099-2120. | 2.0 | 5 |
| 14203 | Effect of 3d heterometallic ions on the magnetic properties of azido-Cu(II) with isonicotinic acid coligands: A theoretical perspective. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 97, 107562. | 1.3 | 11 |
| 14204 | Microhydration of verbenone: how the chain of water molecules adapts its structure to the host molecule. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5855-5864. | 1.3 | 11 |
| 14205 | Initial-state preparation effects in time-resolved electron paramagnetic resonance experiments. <i>Journal of Chemical Physics</i> , 2020, 152, 044304. | 1.2 | 2 |
| 14206 | Profiling C4N radicals of astrophysical interest. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020, 493, 2506-2510. | 1.6 | 8 |
| 14207 | Double hybrids and timeâ€‘dependent density functional theory: An implementation and benchmark on charge transfer excited states. <i>Journal of Computational Chemistry</i> , 2020, 41, 1242-1251. | 1.5 | 42 |
| 14208 | Long Rotational Coherence Times of Molecules in a Magnetic Trap. <i>Physical Review Letters</i> , 2020, 124, 063001. | 2.9 | 28 |
| 14209 | Deriving a Polarizable Force Field for Biomolecular Building Blocks with Minimal Empirical Calibration. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1628-1636. | 1.2 | 8 |
| 14210 | A mechanistic insight into rhodium-doped gold clusters as a better hydrogenation catalyst. <i>Nanoscale</i> , 2020, 12, 5125-5138. | 2.8 | 6 |
| 14211 | Efficient Perovskite Solar Cells by Reducing Interfaceâ€‘Mediated Recombination: a Bulky Amine Approach. <i>Advanced Energy Materials</i> , 2020, 10, 2000197. | 10.2 | 198 |
| 14212 | Catalytic synthesis of bioactive 2H-chromene alcohols from (âˆ‘)-isopulegol and acetone on sulfonated clays. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2020, 129, 627-644. | 0.8 | 9 |
| 14213 | Detection of thiabendazole fungicide/parasiticide by SERS: Quantitative analysis and adsorption mechanism. <i>Applied Surface Science</i> , 2020, 517, 145786. | 3.1 | 53 |
| 14214 | Spectroscopy characterization, theoretical study and antioxidant activities of the flavonoids-Pb(II) complexes. <i>Journal of Molecular Structure</i> , 2020, 1209, 127919. | 1.8 | 22 |
| 14215 | Si₂C₅H₂ isomers â€‘ search algorithms<i> versus</i> chemical intuition. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5865-5872. | 1.3 | 19 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 14216 | Synthesis, characterization, structures and in vitro antitumor activity of platinum(II) complexes bearing adeninato or methylated adeninato ligands. <i>Inorganica Chimica Acta</i> , 2020, 507, 119539. | 1.2 | 1 |
| 14217 | Synthesis and Conformational Analysis of Parent Perhydroazulenes Reveal an Energetically Preferred cis Ring Fusion. <i>Journal of Organic Chemistry</i> , 2020, 85, 4441-4447. | 1.7 | 9 |
| 14218 | Carbon dots derived from human hair for ppb level chloroform sensing in water. <i>Sustainable Materials and Technologies</i> , 2020, 25, e00159. | 1.7 | 21 |
| 14219 | Catalytic Approach toward Chiral P,N-Chelate Complexes Utilizing the Asymmetric Hydrophosphination Protocol. <i>Inorganic Chemistry</i> , 2020, 59, 3874-3886. | 1.9 | 14 |
| 14220 | Development of Density Functional Tight-Binding Parameters Using Relative Energy Fitting and Particle Swarm Optimization. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1469-1481. | 2.3 | 7 |
| 14221 | Formation of Toxic Unsaturated Multifunctional and Organosulfur Compounds From the Photosensitized Processing of Fluorene and DMSO at the Air-Water Interface. <i>Journal of Geophysical Research D: Atmospheres</i> , 2020, 125, e2019JD031839. | 1.2 | 19 |
| 14222 | Color-specific porosity in double pigmented natural 3d-nanoarchitectures of blue crab shell. <i>Scientific Reports</i> , 2020, 10, 3019. | 1.6 | 21 |
| 14223 | Shedding light on the bonding situation of triangular and square heterometallic clusters: computational insight. <i>New Journal of Chemistry</i> , 2020, 44, 5079-5087. | 1.4 | 2 |
| 14224 | Tuning of the redox potential and catalytic activity of a new Cu(II) complex byo-iminobenzosemiquinone as an electron-reservoir ligand. <i>New Journal of Chemistry</i> , 2020, 44, 4426-4439. | 1.4 | 11 |
| 14225 | Cyclic Aminosilane-Based Additive Ensuring Stable Electrode-Electrolyte Interfaces in Li-Ion Batteries. <i>Advanced Energy Materials</i> , 2020, 10, 2000012. | 10.2 | 91 |
| 14226 | Oriented (Local) Electric Fields Drive the Millionfold Enhancement of the H-Abstraction Catalysis Observed for Synthetic Metalloenzyme Analogues. <i>Angewandte Chemie</i> , 2020, 132, 7989-7994. | 1.6 | 8 |
| 14227 | Accurate Prediction of Gas Chromatographic Retention Times via Density Functional Theory Calculations: A Case Study Using Brominated Flame Retardants. <i>ChemistrySelect</i> , 2020, 5, 2476-2481. | 0.7 | 1 |
| 14228 | Nonrelativistic protocol for calculating the 1J(195Pt-15N) coupling constant in Pt(II)-complexes using all-electron Gaussian basis-set. <i>Chemical Physics Letters</i> , 2020, 745, 137279. | 1.2 | 9 |
| 14229 | The effect of CF ₃ functional group substituent on bifunctional activation model and enantioselectivity for BINOL N-triflylphosphoramides catalyzed rearrangement reaction. <i>Journal of Catalysis</i> , 2020, 383, 230-238. | 3.1 | 9 |
| 14230 | SERS and DFT Study of Noble-Metal-Anchored Cys-Trp/Trp-Cys Dipeptides: Influence of Main-Chain Direction and Terminal Modifications. <i>Journal of Physical Chemistry C</i> , 2020, 124, 7097-7116. | 1.5 | 16 |
| 14231 | Predicting Core Level Photoelectron Spectra of Amino Acids Using Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2256-2262. | 2.1 | 11 |
| 14232 | Visible-Light-Induced Metal-/Photocatalyst-Free C-H Bond Imidation of Arenes. <i>Organic Letters</i> , 2020, 22, 2235-2239. | 2.4 | 23 |
| 14233 | Extensive Quantum Chemistry Study of Neutral and Charged C ₄ N Chains: An Attempt To Aid Astronomical Observations. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 434-448. | 1.2 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14234 | Density Functional Theory Calculation on the Structural, Electronic, and Optical Properties of Fluorene-Based Azo Compounds. <i>ACS Omega</i> , 2020, 5, 4507-4531. | 1.6 | 16 |
| 14235 | Electronic-level insight into the weak interactions of ion pairs in acetate anion-based ionic liquids. <i>Journal of Molecular Liquids</i> , 2020, 303, 112668. | 2.3 | 10 |
| 14236 | Sub-picosecond charge-transfer at near-zero driving force in polymer:non-fullerene acceptor blends and bilayers. <i>Nature Communications</i> , 2020, 11, 833. | 5.8 | 130 |
| 14237 | Chitosan oligosaccharide derived polar host for lithium deposition in lithium metal batteries. <i>Sustainable Materials and Technologies</i> , 2020, 24, e00158. | 1.7 | 10 |
| 14238 | Heteronuclear Iron(III)–Schiff Base Complexes with the Hexacyanidocobaltate(III) Anion: On the Quest To Understand the Governing Factors of Spin Crossover. <i>Inorganic Chemistry</i> , 2020, 59, 2747-2757. | 1.9 | 10 |
| 14239 | Quantum Chemical Investigation of Dimerization in the Schlenk Equilibrium of Thiophene Grignard Reagents. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1480-1488. | 1.1 | 7 |
| 14240 | Electronic State of Low-Rank Coals with Exchanged Sodium Cations. <i>ACS Omega</i> , 2020, 5, 1688-1697. | 1.6 | 1 |
| 14241 | Mapping the optoelectronic property space of small aromatic molecules. <i>Communications Chemistry</i> , 2020, 3, . | 2.0 | 14 |
| 14242 | 17.1% Efficient Single-Junction Organic Solar Cells Enabled by n-Type Doping of the Bulk-Heterojunction. <i>Advanced Science</i> , 2020, 7, 1903419. | 5.6 | 173 |
| 14243 | Principle of progressively and strongly immobilizing polysulfides on polyoxovanadate clusters for excellent Li–S batteries application. <i>Nano Energy</i> , 2020, 71, 104596. | 8.2 | 15 |
| 14244 | Photoabsorption, photoionization, and Auger processes at the carbon K edge in CH ₃ I. <i>Physical Review A</i> , 2020, 101, . | 1.0 | 7 |
| 14245 | Infrared Spectroelectrochemistry of Iron-Nitrosyl Triarylcorroles. Implications for Ligand Noninnocence. <i>Inorganic Chemistry</i> , 2020, 59, 3232-3238. | 1.9 | 12 |
| 14246 | Aqueous-Phase Conformations of Lactose, Maltose, and Sucrose and the Assessment of Low-Cost DFT Methods with the DSCONF Set of Conformers for the Three Disaccharides. <i>Journal of Physical Chemistry A</i> , 2020, 124, 582-590. | 1.1 | 20 |
| 14247 | Singlet oxygen stimulus for switchable functional organic cages. <i>Chemical Science</i> , 2020, 11, 1478-1484. | 3.7 | 25 |
| 14248 | Nonsphericity in diferratetracarboranes having 2 <i>n</i> + 2 Wadean skeletal electrons: deviations from <i>closo</i> Δ polyhedral geometries and high-energy kinetically stable isomers. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 2437-2448. | 1.3 | 1 |
| 14249 | Rational Development of Remote C–H Functionalization of Biphenyl: Experimental and Computational Studies. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 4770-4777. | 7.2 | 39 |
| 14250 | Clar Rules the Electronic Properties of 2D π -Conjugated Frameworks: Mind the Gap. <i>Chemistry - A European Journal</i> , 2020, 26, 6569-6575. | 1.7 | 8 |
| 14251 | Cooperative Donor–Acceptor Interactions in Stabilizing Carbene–Borane and Carbene–Alane Compounds: A Theoretical Insight. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 638-655. | 1.0 | 14 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14252 | Relativistic DFT Calculations of $1J_{WH}$ and $1J_{WC}$ Provide Detailed Structural Insight of Cyclopentadienyl Binding in Cp_2WH_2 . <i>Journal of Physical Chemistry A</i> , 2020, 124, 966-975. | 1.1 | 1 |
| 14253 | Feasibility of pristine, Al-doped and Ga-doped Boron Nitride nanotubes for detecting SF ₄ gas: A DFT, NBO and QTAIM investigation. <i>Applied Surface Science</i> , 2020, 510, 145490. | 3.1 | 63 |
| 14254 | Organic Light-Emitting Diode Employing Metal-Free Organic Phosphor. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 6137-6143. | 4.0 | 35 |
| 14255 | Design of single-porphyrin donors toward high open-circuit voltage for organic solar cells via an energy level gradient-distribution screening strategy of fragments: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4015-4022. | 1.3 | 7 |
| 14256 | Excited-state intramolecular proton transfer driven by conical intersection in hydroxychromones. <i>Journal of Computational Chemistry</i> , 2020, 41, 1068-1080. | 1.5 | 11 |
| 14257 | Discovering seminal works with marker papers. <i>Scientometrics</i> , 2020, 125, 2955-2969. | 1.6 | 7 |
| 14258 | Are Heterometallapentalenes Aromatic or Not? A DFT Investigation. <i>Chemistry - A European Journal</i> , 2020, 26, 5381-5387. | 1.7 | 4 |
| 14259 | Mechanisms of Orthogonal Photodecarbonylation Reactions of 3-Hydroxyflavone-Based Acid-Base Forms. <i>Journal of Organic Chemistry</i> , 2020, 85, 3527-3537. | 1.7 | 27 |
| 14260 | Expanded Coumarins: One-Pot Photo Synthesis of 5-Hydroxy-Benzo[12,1]tetrapheno[7,6,5-cde]chromen-5-ones and Photophysical Properties. <i>Journal of Organic Chemistry</i> , 2020, 85, 3689-3698. | 1.7 | 23 |
| 14261 | Negative Electron Affinities and Derivative Discontinuity Contribution from a Generalized Gradient Approximation Exchange Functional. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1334-1342. | 1.1 | 6 |
| 14262 | Catalyst Design for Alkene Epoxidation by Molecular Analogues of Heterogeneous Titanium-Silicalite Catalysts. <i>ACS Catalysis</i> , 2020, 10, 4737-4750. | 5.5 | 45 |
| 14263 | Predicting the Thermodynamic Stability of Zirconium Radiotracers. <i>Inorganic Chemistry</i> , 2020, 59, 2070-2082. | 1.9 | 44 |
| 14264 | Unusual demetalation of iron from [2]ferrocenophane skeleton of dinuclear ferracycle carbonyl complex. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5431. | 1.7 | 1 |
| 14265 | Tributyltin(IV) ferulate, a novel synthetic ferulic acid derivative, induces autophagic cell death in colon cancer cells: From chemical synthesis to biochemical effects. <i>Journal of Inorganic Biochemistry</i> , 2020, 205, 110999. | 1.5 | 36 |
| 14266 | Enhancing triplet sensitization ability of donor-acceptor dyads via intramolecular triplet energy transfer. <i>Journal of Materials Chemistry C</i> , 2020, 8, 3536-3544. | 2.7 | 15 |
| 14267 | Removal of food dyes from aqueous solution by chitosan-vermiculite beads. <i>International Journal of Biological Macromolecules</i> , 2020, 148, 635-646. | 3.6 | 48 |
| 14268 | Rhodium-catalyzed ene-cycloisomerization of allylic-sulfide-tethered alkylidenecyclopropanes: DFT analysis of origins of regio- and diastereo-selectivities. <i>Organic Chemistry Frontiers</i> , 2020, 7, 678-688. | 2.3 | 6 |
| 14269 | Orbital localization error of density functional theory in shear properties of vanadium and niobium. <i>Journal of Chemical Physics</i> , 2020, 152, 024118. | 1.2 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14270 | Solvation structure and molecular interactions of ibuprofen with ethanol and water: A theoretical study. <i>Fluid Phase Equilibria</i> , 2020, 510, 112454. | 1.4 | 20 |
| 14271 | Magnetic anisotropy in Cr ₂ GeC investigated by X-ray magnetic circular dichroism and ab initio calculations. <i>Journal of Magnetism and Magnetic Materials</i> , 2020, 501, 166470. | 1.0 | 5 |
| 14272 | Time-Dependent Density Functional Theory Investigation of Excited State Intramolecular Proton Transfer in Tris(2-hydroxyphenyl)triazasumanene. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1227-1234. | 1.1 | 13 |
| 14273 | Unusual Behavior of the Bipolar Molecule 25-Hydroxycholesterol at the Air/Water Interface—Langmuir Monolayer Approach Complemented with Theoretical Calculations. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1104-1114. | 1.2 | 15 |
| 14274 | Evidence That Molecules in Molecular Junctions May Not Be Subject to the Entire External Perturbation Applied to Electrodes. <i>Langmuir</i> , 2020, 36, 1329-1337. | 1.6 | 5 |
| 14275 | Unveiling the Delicate Balance of Steric and Dispersion Interactions in Organocatalysis Using High-Level Computational Methods. <i>Journal of the American Chemical Society</i> , 2020, 142, 3613-3625. | 6.6 | 58 |
| 14276 | Anharmonic kinetics of the cyclopentane reaction with hydroxyl radical. <i>Chemical Science</i> , 2020, 11, 2511-2523. | 3.7 | 20 |
| 14277 | Electrochemical characterization of the artificial metalloenzyme papain-[(<i>l</i> -6-arene)Ru(1,10-phenanthroline)Cl] ⁺ . <i>Journal of Electroanalytical Chemistry</i> , 2020, 859, 113882. | 1.9 | 1 |
| 14278 | Synthetic Strategies for Trapping the Elusive <i>trans</i> -Dirhodium(II,II) Formamidinate Isomer: Effects of Cis versus Trans Geometry on the Photophysical Properties. <i>Inorganic Chemistry</i> , 2020, 59, 2255-2265. | 1.9 | 1 |
| 14279 | Palladium-Mediated CO ₂ Extrusion Followed by Insertion of Isocyanates for the Synthesis of Benzamides: Translating Fundamental Mechanistic Studies To Develop a Catalytic Protocol. <i>Organometallics</i> , 2020, 39, 453-467. | 1.1 | 17 |
| 14280 | Toolbox approach for quasi-relativistic calculation of molecular properties for precision tests of fundamental physics. <i>Journal of Chemical Physics</i> , 2020, 152, 044101. | 1.2 | 17 |
| 14281 | Heat capacity and decomposition of rimantadine hydrochloride. <i>Thermochimica Acta</i> , 2020, 686, 178538. | 1.2 | 1 |
| 14282 | Metal self-assembly mimosine peptides with enhanced antimicrobial activity: towards a new generation of multitasking chelating agents. <i>Dalton Transactions</i> , 2020, 49, 2862-2879. | 1.6 | 13 |
| 14283 | Restricted Ion Transport by Plasticizing Side Chains in Polycarbonate-Based Solid Electrolytes. <i>Macromolecules</i> , 2020, 53, 764-774. | 2.2 | 42 |
| 14284 | Dilution of the Electron Density in the π -Conjugated Skeleton of Organic Cathode Materials Improves the Discharge Voltage. <i>ChemSusChem</i> , 2020, 13, 2264-2270. | 3.6 | 34 |
| 14285 | Selective Hydrogenation of Acetylene Catalysed by a B ₁₂ N ₁₂ Cluster Doped with a Single Nickel Atom: A DFT Study. <i>Catalysts</i> , 2020, 10, 115. | 1.6 | 7 |
| 14286 | A 2D covalent organic framework as a high-performance cathode material for lithium-ion batteries. <i>Nano Energy</i> , 2020, 70, 104498. | 8.2 | 144 |
| 14287 | Global aromaticity at the nanoscale. <i>Nature Chemistry</i> , 2020, 12, 236-241. | 6.6 | 121 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14288 | Tuning Second-Order Nonlinear Optical Properties of Cross-Linked Carbon Nanotube via External Electric Field. <i>Journal of Physical Chemistry C</i> , 2020, 124, 3778-3783. | 1.5 | 10 |
| 14289 | Rational Development of Remote C-H Functionalization of Biphenyl: Experimental and Computational Studies. <i>Angewandte Chemie</i> , 2020, 132, 4800-4807. | 1.6 | 3 |
| 14290 | A simple method of identifying π orbitals for non-planar systems and a protocol of studying π electronic structure. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1. | 0.5 | 171 |
| 14291 | PiNN: A Python Library for Building Atomic Neural Networks of Molecules and Materials. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1184-1193. | 2.5 | 48 |
| 14292 | An experimental and molecular dynamics simulation study of the structural and thermodynamic properties of the binary mixtures of morpholine and propylene glycol. <i>Journal of Molecular Liquids</i> , 2020, 302, 112584. | 2.3 | 10 |
| 14293 | Microwave Spectrum and Internal Rotations of Heptan-2-one: A Pheromone in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1353-1361. | 1.1 | 18 |
| 14294 | Preserving Symmetry and Degeneracy in the Localized Orbital Scaling Correction Approach. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1528-1535. | 2.1 | 31 |
| 14295 | Chain-Increment Method for Free-Energy Computation of a Polymer with All-Atom Molecular Simulations. <i>Macromolecules</i> , 2020, 53, 775-788. | 2.2 | 11 |
| 14296 | 6-Deoxy-6-fluoro galactofuranosides: regioselective glycosylation, unexpected reactivity, and anti-leishmanial activity. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 1462-1475. | 1.5 | 3 |
| 14297 | Solvent-Mediated Chemical Hole Doping of Graphene by Iodine. <i>Journal of Physical Chemistry C</i> , 2020, 124, 3827-3834. | 1.5 | 5 |
| 14298 | Lignin solvation by ionic liquids: The role of cation. <i>Journal of Molecular Liquids</i> , 2020, 303, 112588. | 2.3 | 17 |
| 14299 | Kinetic modelling of acyl glucuronide and glucoside reactivity and development of structure-property relationships. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 1389-1401. | 1.5 | 5 |
| 14300 | The combination of multipartitioning of the Hamiltonian with canonical Van Vleck perturbation theory leads to a Hermitian variant of quasidegenerate N-electron valence perturbation theory. <i>Journal of Chemical Physics</i> , 2020, 152, 014109. | 1.2 | 10 |
| 14301 | Ionic-caged heterometallic bismuth-platinum complex exhibiting electrocatalytic CO ₂ reduction. <i>Dalton Transactions</i> , 2020, 49, 2652-2660. | 1.6 | 9 |
| 14302 | Comprehensive Insights into the Catalytic Mechanism of Middle East Respiratory Syndrome 3C-Like Protease and Severe Acute Respiratory Syndrome 3C-Like Protease. <i>ACS Catalysis</i> , 2020, 10, 5871-5890. | 5.5 | 78 |
| 14303 | A third-order nonlinear optical single crystal of 3,4-dimethoxy-substituted chalcone derivative with high laser damage threshold value: a potential material for optical power limiting. <i>Journal of Materials Science: Materials in Electronics</i> , 2020, 31, 9133-9150. | 1.1 | 31 |
| 14304 | Determination of the molecular size from measurements of vapour pressure of binary liquid mixtures. Theory, experiments and quantum chemical calculations. <i>Journal of Molecular Liquids</i> , 2020, 313, 113202. | 2.3 | 2 |
| 14305 | Designing Novel High-Performance Shale Inhibitors by Optimizing the Spacer Length of Imidazolium-Based Bola-Form Ionic Liquids. <i>Energy & Fuels</i> , 2020, 34, 5838-5845. | 2.5 | 19 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14306 | Xe ⁺ OCS: relatively straightforward?. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5615-5624. | 1.3 | 4 |
| 14307 | Lithium bis(oxalate)borate additive in the electrolyte to improve Li-rich layered oxide cathode materials. <i>Materials Chemistry Frontiers</i> , 2020, 4, 1689-1696. | 3.2 | 33 |
| 14308 | Chromatographic resolution of phenylethanolic-azole racemic compounds highlighted stereoselective inhibition of heme oxygenase-1 by (R)-enantiomers. <i>Bioorganic Chemistry</i> , 2020, 99, 103777. | 2.0 | 11 |
| 14309 | Bayesian Optimization for Calibrating and Selecting Hybrid-Density Functional Models. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4053-4061. | 1.1 | 107 |
| 14310 | New Zn(II) coordination polymer of indole-3-acetic acid, a plant-growth promoting hormone: Crystal structure, spectroscopic characterization, DFT calculations and microbiological activity. <i>Polyhedron</i> , 2020, 185, 114582. | 1.0 | 6 |
| 14311 | Status and Challenges of Density Functional Theory. <i>Trends in Chemistry</i> , 2020, 2, 302-318. | 4.4 | 216 |
| 14312 | Structure Elucidation of Prenyl- and Geranyl-Substituted Coumarins in <i>Gerbera piloselloides</i> by NMR Spectroscopy, Electronic Circular Dichroism Calculations, and Single Crystal X-ray Crystallography. <i>Molecules</i> , 2020, 25, 1706. | 1.7 | 12 |
| 14313 | Diborane(4) Azides: Surprisingly Stable Sources of Transient Iminoboranes. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15480-15486. | 7.2 | 21 |
| 14314 | Antiproliferative Evaluation of Some 2-((2-Phenylethenyl)cyclopent-3-en-1-yl)acetyl-3-benzothiazoles: DFT and Molecular Docking Study. <i>Chemistry and Biodiversity</i> , 2020, 17, e1900675. | 1.0 | 9 |
| 14315 | Salen-Based Conjugated Microporous Polymers for Efficient Oxygen Evolution Reaction. <i>Chemistry - A European Journal</i> , 2020, 26, 7720-7726. | 1.7 | 16 |
| 14316 | A Systems Approach to a One-Pot Electrochemical Wittig Olefination Avoiding the Use of Chemical Reductant or Sacrificial Electrode. <i>Chemistry - A European Journal</i> , 2020, 26, 11829-11834. | 1.7 | 18 |
| 14317 | Analysis of environment response effects on excitation energies within subsystem-based time-dependent density-functional theory. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26213. | 1.0 | 22 |
| 14318 | Syntheses, solution behavior, and computational bond length analyses of trifluoromethyl and perfluoroethyl cuprate salts. <i>Journal of Fluorine Chemistry</i> , 2020, 234, 109518. | 0.9 | 5 |
| 14319 | Reactivity of eumelanin building blocks: A DFT study of monomers and dimers. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 98, 107609. | 1.3 | 22 |
| 14320 | Crystal structure, FT-Raman and FTIR spectra and DFT calculations of chalcone (2E)-1-(4-aminophenyl)-3-(furan-2-yl)prop-2-en-1-one monohydrate. <i>Journal of Molecular Structure</i> , 2020, 1212, 128141. | 1.8 | 14 |
| 14321 | Tailoring Dihydroxyphthalazines to Enable Their Stable and Efficient Use in the Catholyte of Aqueous Redox Flow Batteries. <i>Chemistry of Materials</i> , 2020, 32, 3427-3438. | 3.2 | 22 |
| 14322 | Effect of Distortions on the Geometric and Electronic Structures of One-Electron Oxidized Vanadium(IV), Copper(II), and Cobalt(II)/(III) Salen Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 5133-5148. | 1.9 | 43 |
| 14323 | The ONIOM/PMM Model for Effective Yet Accurate Simulation of Optical and Chiroptical Spectra in Solution: Camphorquinone in Methanol as a Case Study. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3294-3306. | 2.3 | 17 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14324 | 6-Deoxy- and 11-Hydroxytolypodiols: Meroterpenoids from the Cyanobacterium HT-58-2. <i>Journal of Natural Products</i> , 2020, 83, 1691-1695. | 1.5 | 8 |
| 14325 | Alkanethiol-Mediated Cyclization of <i>o</i> -Alkynylisocyanobenzenes: Synthesis of Bis-Thiolated Indole Derivatives. <i>Journal of Organic Chemistry</i> , 2020, 85, 6338-6351. | 1.7 | 14 |
| 14326 | Stereoselective Synthesis of (<i>E</i>)-3-Alkylideneoxindoles via Gold(I)-Catalyzed Cross-Coupling of 3-Diazooxindoles with Diazoesters. <i>Journal of Organic Chemistry</i> , 2020, 85, 5863-5871. | 1.7 | 9 |
| 14327 | Impact of Cyanine Conformational Restraint in the Near-Infrared Range. <i>Journal of Organic Chemistry</i> , 2020, 85, 5907-5915. | 1.7 | 60 |
| 14328 | Second Near-Infrared Aggregation-Induced Emission Fluorophores with Phenothiazine Derivatives as the Donor and 6,7-Diphenyl-[1,2,5]Thiadiazolo[3,4-g]Quinoxaline as the Acceptor for In Vivo Imaging. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 20281-20286. | 4.0 | 36 |
| 14329 | An anthracene-pendant ruthenium(II) complex conjugated to a biotin anchor, an essential handle for photo-induced anti-cancer activity. <i>New Journal of Chemistry</i> , 2020, 44, 6610-6622. | 1.4 | 9 |
| 14330 | Theoretical study of the mechanism behind the site- and enantio-selectivity of C-H functionalization catalysed by chiral dirhodium catalyst. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9561-9572. | 1.3 | 5 |
| 14331 | Oxidative Rearrangement via 1,2-Aryl Migration using Hydroxy(tosyloxy)iodobenzene in a Polar Aprotic Solvent. <i>Synlett</i> , 2020, 31, 959-964. | 1.0 | 9 |
| 14332 | New Cysteine Protease Inhibitors: Electrophilic (Het)arenes and Unexpected Prodrug Identification for the Trypanosoma Protease Rhodessain. <i>Molecules</i> , 2020, 25, 1451. | 1.7 | 16 |
| 14333 | Two Simple and Highly Efficient Variants of the Griffith-Ley Oxidation of Alcohols. <i>ChemCatChem</i> , 2020, 12, 3919-3928. | 1.8 | 6 |
| 14334 | Are Heterometallapentalenes Aromatic or Not? A DFT Investigation. <i>Chemistry - A European Journal</i> , 2020, 26, 5307-5307. | 1.7 | 1 |
| 14335 | 3-Methyl-4-thio-1 <i>H</i> -tetrahydropyranspiro-5,5-dihydro-2H-chrydantoin platinum complex as a novel potent anticancer agent and xanthine oxidase inhibitor. <i>Archiv Der Pharmazie</i> , 2020, 353, e2000039. | 2.1 | 9 |
| 14336 | Synthesis, Photophysical and Electronic Properties of Mono-, Di-, and Tri-Amino-Substituted Ortho-Perylenes, and Comparison to the Tetra-Substituted Derivative. <i>Chemistry - A European Journal</i> , 2020, 26, 12050-12059. | 1.7 | 8 |
| 14337 | Arsenic-nucleotides interactions: an experimental and computational investigation. <i>Dalton Transactions</i> , 2020, 49, 6302-6311. | 1.6 | 10 |
| 14338 | How accurate are TD-DFT excited state geometries compared to DFT ground state geometries?. <i>Journal of Computational Chemistry</i> , 2020, 41, 1718-1729. | 1.5 | 57 |
| 14339 | [Mo ₂ O ₂ S ₈] ²⁻ small molecule dimer as a basis for hydrogen evolution reaction (HER) catalyst materials. <i>SN Applied Sciences</i> , 2020, 2, 1. | 1.5 | 8 |
| 14340 | Performance of Localized Coupled Cluster Methods in a Moderately Strong Correlation Regime: H ₄ chelating-Möbius Interconversions in Expanded Porphyrins. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3641-3653. | 2.3 | 44 |
| 14341 | Cyclometalated Ir(III) complexes as tuneable multiband light sources for optical multisensor systems: Feasibility study. <i>Dyes and Pigments</i> , 2020, 180, 108428. | 2.0 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14342 | Spectroscopic characterization and efflux pump modulation of a thiophene curcumin derivative. <i>Journal of Molecular Structure</i> , 2020, 1215, 128291. | 1.8 | 17 |
| 14343 | Prediction of Solvation Free Energies of Ionic Solutes in Neutral Solvents. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4171-4181. | 1.1 | 15 |
| 14344 | Establishing best practices to model the electronic structure of CuFeO_2 from first principles. <i>Physical Review B</i> , 2020, 101, . | | |
| 14345 | Eutectics and Salt of Dapsone With Hydroxybenzoic Acids: Binary Phase Diagrams, Characterization and Evaluation. <i>Journal of Pharmaceutical Sciences</i> , 2020, 109, 2224-2236. | 1.6 | 12 |
| 14346 | Copper(I) halide polymers derived from tris[2-(pyridin-2-yl)ethyl]phosphine: halogen-tunable colorful luminescence spanning from deep blue to green. <i>New Journal of Chemistry</i> , 2020, 44, 6916-6922. | 1.4 | 31 |
| 14347 | Rapid Raman Spectroscopic Analysis of Stress Induced Degradation of the Pharmaceutical Drug Tetracycline. <i>Molecules</i> , 2020, 25, 1866. | 1.7 | 6 |
| 14348 | What are the effects of cucurbit[<i>n</i>]uril on CTMS loading? Insights from QM calculations and MD simulations. <i>Computational Materials Science</i> , 2020, 181, 109751. | 1.4 | 5 |
| 14349 | Development of an Unsymmetrical Cyclopropenimine-Guanidine Platform for Accessing Strongly Basic Proton Sponges and Boron-Difluoride Diaminonaphthalene Fluorophores. <i>Chemistry - A European Journal</i> , 2020, 26, 8608-8620. | 1.7 | 9 |
| 14350 | Balancing Density Functional Theory Interaction Energies in Charged Dimers Precursors to Organic Semiconductors. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3530-3542. | 2.3 | 2 |
| 14351 | Direct Synthesis of the Phenanthroviridone Skeleton Using a Highly Regioselective Nitroquinone Diels-Alder Reaction. <i>ACS Omega</i> , 2020, 5, 9311-9315. | 1.6 | 2 |
| 14352 | Wannier-Koopmans method calculations for transition metal oxide band gaps. <i>Npj Computational Materials</i> , 2020, 6, . | 3.5 | 11 |
| 14353 | A long-chain based bromo and methyl substituted chalcone derivatives; experimental and theoretical approach on nonlinear optical single crystals. <i>Materials Research Express</i> , 2020, 7, 055101. | 0.8 | 15 |
| 14354 | Double hybrid DFT calculations with Slater type orbitals. <i>Journal of Computational Chemistry</i> , 2020, 41, 1660-1684. | 1.5 | 16 |
| 14355 | Hybrid functionals with system-dependent parameters: Conceptual foundations and methodological developments. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1476. | 6.2 | 7 |
| 14356 | A theoretical investigation on the mechanism and kinetics of the thermal isomerization of Trimethylsilylcyclopropane using CBS-QB3. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2020, 130, 55-74. | 0.8 | 3 |
| 14357 | Three-component coupling reaction of the C60 fullerene, indole and propargyl bromide: a theoretical study. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2020, 130, 75-90. | 0.8 | 4 |
| 14358 | Azo dye aggregates and their roles in the morphology and conductivity of polypyrrole. <i>Dyes and Pigments</i> , 2020, 177, 108329. | 2.0 | 18 |
| 14359 | 9-Ethyladenine: Mechanochemical Synthesis, Characterization, and DFT Calculations of Novel Cocrystals and Salts. <i>Crystal Growth and Design</i> , 2020, 20, 2985-2997. | 1.4 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14360 | Atomic Layer Deposition of Localized Boron- and Hydrogen-Doped Aluminum Oxide Using Trimethyl Borate as a Dopant Precursor. <i>Chemistry of Materials</i> , 2020, 32, 4152-4165. | 3.2 | 2 |
| 14361 | Versatile Coordination Chemistry of Hexa-tert-butyl-octaphosphine. <i>Inorganic Chemistry</i> , 2020, 59, 7487-7503. | 1.9 | 7 |
| 14362 | Stronger Hydration of Eu(III) Impedes Its Competition against Am(III) in Binding with N-donor Extractants. <i>Inorganic Chemistry</i> , 2020, 59, 6267-6278. | 1.9 | 15 |
| 14363 | Approximate versus Exact Embedding for Chiroptical Properties: Reconsidering Failures in Potential and Response. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3104-3120. | 2.3 | 18 |
| 14364 | Calculation of Anharmonic IR and Raman Intensities for Periodic Systems from DFT Calculations: Implementation and Validation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3343-3351. | 2.3 | 7 |
| 14365 | On the Spectroscopic Modeling of Localized Defects in Sodalites by TD-DFT. <i>Journal of Physical Chemistry C</i> , 2020, 124, 8949-8957. | 1.5 | 15 |
| 14366 | Structure-Property Relationships in Sterically Congested Proton-Conducting Poly(phenylene)s: the Impact of Biphenyl Linearity. <i>Macromolecules</i> , 2020, 53, 3119-3138. | 2.2 | 26 |
| 14367 | Fluorescence and Optical Activity of Chiral CdTe Quantum Dots in Their Interaction with Amino Acids. <i>ACS Nano</i> , 2020, 14, 4196-4205. | 7.3 | 53 |
| 14368 | Too Persistent to Give Up: Aromaticity in Boron Clusters Survives Radical Structural Changes. <i>Journal of the American Chemical Society</i> , 2020, 142, 9396-9407. | 6.6 | 145 |
| 14369 | Non-bonded force field model with advanced restrained electrostatic potential charges (RESP2). <i>Communications Chemistry</i> , 2020, 3, . | 2.0 | 98 |
| 14370 | <i>Ab initio</i> study on the excited states of pyrene and its derivatives using multi-reference perturbation theory methods. <i>RSC Advances</i> , 2020, 10, 12988-12998. | 1.7 | 11 |
| 14371 | Dehydrogenation of amines in aryl-amine functionalized pincer-like nitrogen-donor redox non-innocent ligands via ligand reduction on a Ni($\text{N}^{\text{C}}\text{N}^{\text{C}}\text{N}^{\text{C}}$) template. <i>Dalton Transactions</i> , 2020, 49, 6816-6831. | 1.6 | 9 |
| 14372 | The competition between dehydrogenation and dehydration reactions for primary and secondary alcohols over gallia: unravelling the effects of molecular and electronic structure via a two-pronged theoretical/experimental approach. <i>Catalysis Science and Technology</i> , 2020, 10, 3433-3449. | 2.1 | 10 |
| 14373 | Systematic description of molecular deformations with Cremer-Pople puckering and deformation coordinates utilizing analytic derivatives: Applied to cycloheptane, cyclooctane, and cyclo[18]carbon. <i>Journal of Chemical Physics</i> , 2020, 152, 154107. | 1.2 | 16 |
| 14374 | Computational study on the electronic g-tensors of hydrophilic and hydrophobic nanodiamonds interacting with water. <i>Journal of Chemical Physics</i> , 2020, 152, 144302. | 1.2 | 2 |
| 14375 | Synthesis, Structural, and Physico-Chemical Study of Transition Metal Complexes with Schiff Base: A Product of Condensation of 2-N-Tosylaminobenzaldehyde and Tryptamine. <i>Russian Journal of General Chemistry</i> , 2020, 90, 418-424. | 0.3 | 0 |
| 14376 | The Antioxidant Peptide Salamandrin-I: First Bioactive Peptide Identified from Skin Secretion of Salamandra Genus (<i>Salamandra salamandra</i>). <i>Biomolecules</i> , 2020, 10, 512. | 1.8 | 22 |
| 14377 | The Activation Strain Model in the Light of Real Space Energy Partitions. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2020, 646, 1062-1072. | 0.6 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14378 | Molecular Recognition and Band Alignment in 3D Covalent Organic Frameworks for Cocrystalline Organic Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2020, 124, 9126-9133. | 1.5 | 14 |
| 14379 | Interatomic Interactions in Heterometallic Cubane-Type Clusters with $\{Mo_3S_4M\} (M = Cu, Ni, Pd)$ Core. <i>Journal of Cluster Science</i> , 2021, 32, 415-421. | 1.7 | 5 |
| 14380 | Gas-Phase Dissociation Chemistry of Deprotonated RGD. <i>Journal of the American Society for Mass Spectrometry</i> , 2021, 32, 55-63. | 1.2 | 4 |
| 14381 | Site-Selective Photoinduced Electron Transfer of Excited-State Intermolecular Hydrogen-Bonded Cluster in Solution. <i>Journal of Cluster Science</i> , 2021, 32, 93-99. | 1.7 | 2 |
| 14382 | Molecular docking, DFT and antimicrobial studies of Cu(II) complex as topoisomerase I inhibitor. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 2092-2105. | 2.0 | 13 |
| 14383 | Insight into the CO ₂ photoreduction mechanism over 9-hydroxyphenal-1-one (HPHN) carbon quantum dots. <i>Journal of Energy Chemistry</i> , 2021, 52, 269-276. | 7.1 | 9 |
| 14384 | High CO ₂ absorption capacity of metal-based ionic liquids: A molecular dynamics study. <i>Green Energy and Environment</i> , 2021, 6, 253-260. | 4.7 | 60 |
| 14385 | Effects of structure and electronic properties of D-π-A organic dyes on photovoltaic performance of dye-sensitized solar cells. <i>Journal of Energy Chemistry</i> , 2021, 54, 208-216. | 7.1 | 37 |
| 14386 | Predicting reactivity to drug metabolism: beyond P450s modelling FMOs and UGTs. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 541-555. | 1.3 | 13 |
| 14387 | Exploring the potential of group III salen complexes for the conversion of CO ₂ under ambient conditions. <i>Catalysis Today</i> , 2021, 375, 324-334. | 2.2 | 54 |
| 14388 | The Trip to the Density Functional Theory Zoo Continues: Making a Case for Time-Dependent Double Hybrids for Excited-State Problems. <i>Australian Journal of Chemistry</i> , 2021, 74, 3. | 0.5 | 39 |
| 14389 | Nicotinic acid derivatives as corrosion inhibitors for mild steel in hydrochloric acid solutions: an experimental and computational chemistry study. <i>Journal of Adhesion Science and Technology</i> , 2021, 35, 63-80. | 1.4 | 21 |
| 14390 | Toward understanding the ionization mechanism of matrix-assisted ionization using mass spectrometry experiment and theory. <i>Rapid Communications in Mass Spectrometry</i> , 2021, 35, e8382. | 0.7 | 13 |
| 14391 | Exploration of nitrogen heterocycle scaffolds for the development of potent human neutrophil elastase inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2021, 29, 115836. | 1.4 | 9 |
| 14392 | Gas chromatography-vacuum ultraviolet spectroscopic analysis of organosilanes. <i>Talanta</i> , 2021, 223, 121781. | 2.9 | 4 |
| 14393 | Quantum chemical investigation of structure and stability conformers (R)-menthenone. <i>Journal of the Chinese Chemical Society</i> , 2021, 68, 551-556. | 0.8 | 2 |
| 14394 | Phase field simulation of anode microstructure evolution of solid oxide fuel cell through Ni(OH) ₂ diffusion. <i>Journal of Power Sources</i> , 2021, 482, 228971. | 4.0 | 14 |
| 14395 | A Series of Green Light Absorbing Organic Photosensitizers Capable of Oxidative Quenching Photocatalysis. <i>ChemPhotoChem</i> , 2021, 5, 51-57. | 1.5 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14396 | Oxidative transformation of 1-naphthylamine in water mediated by different environmental black carbons. <i>Journal of Hazardous Materials</i> , 2021, 403, 123594. | 6.5 | 5 |
| 14397 | Fitting elephants in the density functionals zoo: Statistical criteria for the evaluation of density functional theory methods as a suitable replacement for counting parameters. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26379. | 1.0 | 7 |
| 14398 | Assessing conformer energies using electronic structure and machine learning methods. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26381. | 1.0 | 40 |
| 14399 | Synthesis, characterisation and comparative study of the hydroxyl, acrylate and vinyl-ether terminated cyanobiphenyl bridged with different spacer lengths. <i>Liquid Crystals</i> , 2021, 48, 168-181. | 0.9 | 2 |
| 14400 | Highly efficient capture of odorous sulfur-based VOCs by ionic liquids. <i>Journal of Hazardous Materials</i> , 2021, 402, 123507. | 6.5 | 20 |
| 14401 | Mechanistic investigation on ethanol to butadiene conversion reaction over metal oxide clusters. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26494. | 1.0 | 13 |
| 14402 | Multiscale Molecular Modelling of ATP-Fueled Supramolecular Polymerisation and Depolymerisation**. <i>ChemSystemsChem</i> , 2021, 3, e2000038. | 1.1 | 8 |
| 14403 | Mechanistic insight into the performance enhancement of Si anode of a lithium-ion battery with a fluoroethylene carbonate electrolyte additive. <i>Journal of Applied Electrochemistry</i> , 2021, 51, 143-154. | 1.5 | 12 |
| 14404 | Effects of zwitterionic surfactant adsorption on the component distribution in the crude oil droplet: A molecular simulation study. <i>Fuel</i> , 2021, 283, 119252. | 3.4 | 36 |
| 14405 | Coordination complexes of di(2-pyridyl)ketone with copper(I) and their formation in solution and under solvent-free conditions. <i>Inorganica Chimica Acta</i> , 2021, 514, 119951. | 1.2 | 5 |
| 14406 | Microscopic mechanism about the selective adsorption of Cr(VI) from salt solution on O-rich and N-rich biochars. <i>Journal of Hazardous Materials</i> , 2021, 404, 124162. | 6.5 | 63 |
| 14407 | A three states model for hydrogen abstraction reactions with the cytochrome P450 compound I is revisited. Isolobal and isospin analogy among Fe(IV)=O, O ²⁻ = \dot{O} and O. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 405, 112902. | 2.0 | 3 |
| 14408 | Synthesis, X-ray and complete assignments of ¹ H and ¹³ C nuclear magnetic resonance data for novel dichloro-1,4-dihydro-1,4-epoxynaphthalene derivatives. <i>Journal of Molecular Structure</i> , 2021, 1224, 129287. | 1.8 | 2 |
| 14409 | Effect of the spin-orbit interaction of ligands on the parameters of EPR spectra for a series of niobium(IV) complexes of trans-[NbX ₄ (OPPh ₃) ₂] (XA=Cl, Br, I). <i>Inorganica Chimica Acta</i> , 2021, 515, 120056. | 1.2 | 2 |
| 14410 | Exploration of adsorption mechanism of 2-phosphonobutane-1,2,4-tricarboxylic acid onto kaolinite and montmorillonite via batch experiment and theoretical studies. <i>Journal of Hazardous Materials</i> , 2021, 403, 123810. | 6.5 | 94 |
| 14411 | Quantification of Noncovalent Interactions in Azide-Pnictogen, Chalcogen, and Halogen Contacts. <i>Chemistry - A European Journal</i> , 2021, 27, 4627-4639. | 1.7 | 25 |
| 14412 | A novel method for the synthesis and characterization of 10-hexyl-3-(1-hexyl-4,)-Tj ETQqO O O rgBT /Overlock 10 Tf 50 107 Td (5-diphenyl) molecular docking studies. <i>Research on Chemical Intermediates</i> , 2021, 47, 759-794. | 1.3 | 12 |
| 14413 | Molecular-level behavior of imidazolium-based ionic liquid mixtures. <i>Chemical Engineering Science</i> , 2021, 229, 116073. | 1.9 | 16 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 14414 | Ab initio investigation of the ground and lowest excited states of the YAl molecule. Computational and Theoretical Chemistry, 2021, 1194, 113057. | 1.1 | 0 |
| 14415 | Role of oxygen functional groups in Pb ²⁺ adsorption from aqueous solution on carbonaceous surface: A density functional theory study. Journal of Hazardous Materials, 2021, 405, 124221. | 6.5 | 15 |
| 14416 | Treatment of ammonia-embodied wastewater by a transition-metal-based photochemical catalysis strategy. Chemosphere, 2021, 270, 128614. | 4.2 | 2 |
| 14417 | Synergistic Size Effect of MOF Cavity/Encapsulated Luminescent Modules Significantly Boosts Nitro-Aromatic Vapors Distinction via a Three-Dimensional Ratiometric Sensing. Sensors and Actuators B: Chemical, 2021, 328, 129025. | 4.0 | 7 |
| 14418 | Relative cross sections and appearance energies in electron impact ionization and dissociation of mono-halogenated biphenyls. International Journal of Mass Spectrometry, 2021, 459, 116452. | 0.7 | 3 |
| 14419 | Reduction and Rearrangement of a Boron(II) Carbonyl Complex. Angewandte Chemie - International Edition, 2021, 60, 2963-2968. | 7.2 | 20 |
| 14420 | Full Spectroscopic Characterization and Cytotoxicity Activity of Synthetic Dibenzalacetone Derivatives. Journal of Molecular Structure, 2021, 1231, 129670. | 1.8 | 2 |
| 14421 | When are two hydrogen bonds better than one? Accurate first-principles models explain the balance of hydrogen bond donors and acceptors found in proteins. Chemical Science, 2021, 12, 1147-1162. | 3.7 | 17 |
| 14422 | Corrosion inhibition of mild steel in acidic medium by simple azole-based aromatic compounds. Journal of Electroanalytical Chemistry, 2021, 880, 114858. | 1.9 | 43 |
| 14423 | Cofactor-free oxidase-mimetic nanomaterials from self-assembled histidine-rich peptides. Nature Materials, 2021, 20, 395-402. | 13.3 | 78 |
| 14424 | Splitting of multiple hydrogen molecules by bioinspired dinitobium metal complexes: a DFT study. Dalton Transactions, 2021, 50, 840-849. | 1.6 | 5 |
| 14425 | Hybrid Peptide-Thiourea Catalyst for Asymmetric Michael Additions of Aldehydes to Heterocyclic Nitroalkenes. Journal of Organic Chemistry, 2021, 86, 581-592. | 1.7 | 8 |
| 14426 | Extended gate-type organic transistor functionalized by molecularly imprinted polymer for taurine detection. Nanoscale, 2021, 13, 100-107. | 2.8 | 22 |
| 14427 | Collisional stabilization of ion-molecule association complexes in He, H ₂ , or N ₂ buffer gases. International Journal of Mass Spectrometry, 2021, 460, 116494. | 0.7 | 2 |
| 14428 | Determination of the absolute solvation free energy and enthalpy of the proton in solutions. Journal of Molecular Liquids, 2021, 322, 114919. | 2.3 | 32 |
| 14429 | First principle study of lithium and phosphorus co-doped graphitic carbon nitride as a nonlinear optical material. Materials Today Communications, 2021, 26, 101911. | 0.9 | 4 |
| 14430 | Isolierung und Reaktivität eines s-Block-Metall-Antiaromaten. Angewandte Chemie, 2021, 133, 3856-3863. | 1.6 | 6 |
| 14431 | Tuning the electrochemical and optical properties of donor-acceptor D-A ₂ -A ₁ -A ₂ -D derivatives with central benzothiadiazole core by changing the A ₂ strength. Electrochimica Acta, 2021, 368, 137540. | 2.6 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 14432 | From antiferromagnetic to ferromagnetic exchange in a family of phenoxido-bridged heterodinuclear Cu(II)-Mn(II) complexes: A magneto-structural theoretical study. <i>Polyhedron</i> , 2021, 194, 114955. | 1.0 | 7 |
| 14433 | Theoretical study of chloride complexes with hybrid macrocycles. <i>New Journal of Chemistry</i> , 2021, 45, 463-470. | 1.4 | 1 |
| 14434 | Molecular single iron site catalysts for electrochemical nitrogen fixation under ambient conditions. <i>Applied Catalysis B: Environmental</i> , 2021, 285, 119794. | 10.8 | 58 |
| 14435 | Refined standards for simulating UV-vis absorption spectra of acceptors in organic solar cells by TD-DFT. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 407, 113087. | 2.0 | 9 |
| 14436 | Structural Changes in Five-coordinate Bromido-bis(o-aminobenzo-semiquinonato)iron(III) Complex: Spin-Crossover or Ligand-Metal Antiferromagnetic Interactions?. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 756-762. | 1.0 | 1 |
| 14437 | Structural and electronic properties of PtnSi12 (n=1-4) clusters: Quantum chemical calculations. <i>Computational and Theoretical Chemistry</i> , 2021, 1195, 113091. | 1.1 | 1 |
| 14438 | Solution and solid-state light-induced transformations in heterometallic vanadium-ruthenium nitrosyl complex. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 407, 113044. | 2.0 | 11 |
| 14439 | Confined Ru-catalysts in a Two-phase Heptane/Ionic Liquid Solution: Modeling Aspects. <i>ChemCatChem</i> , 2021, 13, 739-746. | 1.8 | 2 |
| 14440 | Initial estimate for minimum energy pathways and transition states using velocities in internal coordinates. <i>Chemical Physics</i> , 2021, 542, 111046. | 0.9 | 2 |
| 14441 | Fluorinated cobalt catalysts and their use in forming narrowly dispersed polyethylene waxes of high linearity and incorporating vinyl functionality. <i>Catalysis Science and Technology</i> , 2021, 11, 656-670. | 2.1 | 17 |
| 14442 | SAMPL7: Host-guest binding prediction by molecular dynamics and quantum mechanics. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 63-77. | 1.3 | 9 |
| 14443 | Global optimization of chemical cluster structures: Methods, applications, and challenges. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26553. | 1.0 | 31 |
| 14444 | Colorimetric metal ion (II) Sensors Based on imine boronic esters functionalized with pyridine. <i>Dyes and Pigments</i> , 2021, 186, 108991. | 2.0 | 7 |
| 14445 | Stabilization mechanism of arsenic-sulfide slag by density functional theory calculation of arsenic-sulfide clusters. <i>Journal of Hazardous Materials</i> , 2021, 410, 124567. | 6.5 | 9 |
| 14446 | Mechanism of transition metal cluster catalysts for hydrogen evolution reaction. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 3484-3492. | 3.8 | 17 |
| 14447 | Synthesis and biological evaluation as well as in silico studies of arylpiperazine-1,2-benzothiazine derivatives as novel anti-inflammatory agents. <i>Bioorganic Chemistry</i> , 2021, 106, 104476. | 2.0 | 16 |
| 14448 | A iridium(III) complex-based "turn-on" fluorescent probe with two recognition site for rapid detection of thiophenol and its application in water samples and human serum. <i>Tetrahedron</i> , 2021, 77, 131738. | 1.0 | 7 |
| 14449 | A theoretical investigation on decarboxylation mechanism of antibiotic para-aminosalicylic acid to highly toxic form meta-aminophenol. <i>Structural Chemistry</i> , 2021, 32, 1053-1060. | 1.0 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 14450 | Isolation and Reactivity of an Antiaromatic s-block Metal Compound. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 3812-3819. | 7.2 | 24 |
| 14451 | Carboxylate-Dominant Oxygen Rich Carbon for Improved Sodium Ion Storage: Synergistic Enhancement of Adsorption and Intercalation Mechanisms. <i>Advanced Energy Materials</i> , 2021, 11, . | 10.2 | 133 |
| 14452 | Evaluation of DNA/BSA interactions and DFT calculations of gold(III), zinc(II) and palladium(II) complexes with triammonium N-dithiocarboxyiminodiacetate. <i>Journal of Molecular Structure</i> , 2021, 1229, 129622. | 1.8 | 5 |
| 14453 | Colorimetric detection of Hg ²⁺ and CH ₃ Hg ⁺ by a novel spirooxazine derivative as a highly sensitive and selective probe. <i>Dyes and Pigments</i> , 2021, 186, 108996. | 2.0 | 14 |
| 14454 | The effect of ligand modification on the structure and electronic spectra of tetraazamacrocyclic complexes Au(III). <i>Journal of Molecular Structure</i> , 2021, 1224, 129162. | 1.8 | 3 |
| 14455 | Rhodium-catalyzed C-H olefination of aromatic acids with unactivated olefins to achieve branched vinylylated or linear allylated product: A theoretical investigation. <i>Molecular Catalysis</i> , 2021, 499, 111295. | 1.0 | 4 |
| 14456 | Structural investigations, quantum mechanical studies on proton and metal affinity and biological activity predictions of selpercatinib. <i>Journal of Molecular Liquids</i> , 2021, 325, 114765. | 2.3 | 18 |
| 14457 | Ferrous to Ferric Transition in Fe-Phthalocyanine Driven by NO ₂ Exposure. <i>Chemistry - A European Journal</i> , 2021, 27, 3526-3535. | 1.7 | 16 |
| 14458 | Green-to-Blue Phosphorescent Iridium(III) Complexes with Near Unitary Quantum Yield. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 601-604. | 1.0 | 4 |
| 14459 | A theoretical study of the potential energy surface for the isomerization reaction of fluoranthene to aceanthrylene: Implications for combustion chemistry. <i>Computational and Theoretical Chemistry</i> , 2021, 1196, 113118. | 1.1 | 1 |
| 14460 | Design strategy for blue thermally activated delayed fluorescence: Position and methyl substitutions. <i>Chemical Physics Letters</i> , 2021, 764, 138260. | 1.2 | 6 |
| 14461 | Structure and EPR investigation of Cu(II) bifluoride complexes with zwitterionic N-hydroxyimidazole ligands. <i>Inorganica Chimica Acta</i> , 2021, 517, 120187. | 1.2 | 6 |
| 14462 | Boosting electrochemical performance of activated carbon by tuning effective pores and synergistic effects of active species. <i>Journal of Colloid and Interface Science</i> , 2021, 587, 290-301. | 5.0 | 30 |
| 14463 | The interaction of half-sandwich (1-5-Cp*)Rh(III) cation with histidine containing peptides and their ternary species with (N,N) bidentate ligands. <i>Journal of Inorganic Biochemistry</i> , 2021, 216, 111330. | 1.5 | 3 |
| 14464 | Using high-throughput virtual screening to explore the optoelectronic property space of organic dyes; finding diketopyrrolopyrrole dyes for dye-sensitized water splitting and solar cells. <i>Sustainable Energy and Fuels</i> , 2021, 5, 704-719. | 2.5 | 15 |
| 14465 | Solid-State Molecular Motions in Organic THz Generators. <i>Advanced Optical Materials</i> , 2021, 9, 2001521. | 3.6 | 15 |
| 14466 | Photocatalyzed Transition-Metal-Free Oxidative Cross-Coupling Reactions of Tetraorganoborates**. <i>Chemistry - A European Journal</i> , 2021, 27, 4322-4326. | 1.7 | 14 |
| 14467 | Carbon nitride/polypyrrole composite supercapacitor: Boosting performance and stability. <i>Electrochimica Acta</i> , 2021, 368, 137570. | 2.6 | 22 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 14468 | Lanthanide nitrate complexes bridged by the bis-tridentate ligand 2,3,5,6-tetra(2-pyridyl)pyrazine: Syntheses, crystal structures, Hirshfeld surface analyses, luminescence properties, DFT calculations, and magnetic behavior. <i>Journal of Luminescence</i> , 2021, 232, 117835. | 1.5 | 9 |
| 14469 | Nitro-Substituted Benzaldehydes in the Generation of Azomethine Ylides and Retro-1,3-Dipolar Cycloadditions. <i>Journal of Organic Chemistry</i> , 2021, 86, 547-558. | 1.7 | 3 |
| 14470 | Fluorescent Imidazo[1,2-a]pyrimidine Compounds as Biocompatible Organic Photosensitizers that Generate Singlet Oxygen: A Potential Tool for Phototheranostics. <i>Chemistry - A European Journal</i> , 2021, 27, 6213-6222. | 1.7 | 5 |
| 14471 | Synthesis, photophysical, and theoretical studies on π -conjugated copolymers based on benzothiadiazole and cyanopyridine acceptor moieties along with other π -bridge units. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4158. | 0.9 | 3 |
| 14472 | Quantum Information and Algorithms for Correlated Quantum Matter. <i>Chemical Reviews</i> , 2021, 121, 3061-3120. | 23.0 | 67 |
| 14473 | Aggregation of coronene: the effect of carboxyl and amine functional groups. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1500-1509. | 1.3 | 2 |
| 14474 | Bioresponsive metal-organic frameworks: Rational design and function. <i>Coordination Chemistry Reviews</i> , 2021, 431, 213682. | 9.5 | 17 |
| 14475 | DFT Mechanistic Study on Palladium-Catalyzed Redox-Neutral Hydroarylation of Unactivated Alkenes with Arylboronic Acids. <i>Asian Journal of Organic Chemistry</i> , 2021, 10, 412-420. | 1.3 | 4 |
| 14476 | Synthesis, Characterization and Theoretical Calculations of a Novel Azo Derivative with In Vitro and In Silico Biological Studies. <i>Arabian Journal for Science and Engineering</i> , 2021, 46, 5567-5581. | 1.7 | 6 |
| 14477 | Design, synthesis and biological activity of 1,4-quinone moiety attached to betulin derivatives as potent DT-diaphorase substrate. <i>Bioorganic Chemistry</i> , 2021, 106, 104478. | 2.0 | 16 |
| 14478 | Summary of DFT calculations coupled with current statistical and/or artificial neural network (ANN) methods to assist experimental NMR data in identifying diastereomeric structures. <i>Tetrahedron Letters</i> , 2021, 71, 152548. | 0.7 | 15 |
| 14479 | First-Principles Calculations on Ni,Fe-Containing Carbon Monoxide Dehydrogenases Reveal Key Stereoelectronic Features for Binding and Release of CO ₂ to/from the C-Cluster. <i>Inorganic Chemistry</i> , 2021, 60, 387-402. | 1.9 | 15 |
| 14480 | Functional separator for promoting lithium ion migration and its mechanism study. <i>Applied Surface Science</i> , 2021, 542, 148661. | 3.1 | 14 |
| 14481 | Removal of Co(II) from Aqueous Solutions by Pyridine Schiff Base-Functionalized Zirconium-Based MOFs: A Combined Experimental and DFT Study on the Effect of <i>ortho</i> -, <i>meta</i> -, and <i>para</i> -Substitution. <i>Journal of Chemical & Engineering Data</i> , 2021, 66, 749-760. | 1.0 | 14 |
| 14482 | Accurate Molecular Geometries in Complex Excited-State Potential Energy Surfaces from Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 357-366. | 2.3 | 8 |
| 14483 | Strong electron affinity PDI supramolecules form anion radicals for the degradation of organic pollutants <i>via</i> direct electrophilic attack. <i>Catalysis Science and Technology</i> , 2021, 11, 1899-1913. | 2.1 | 7 |
| 14484 | NH ₃ separation membranes with self-assembled gas highways induced by protic ionic liquids. <i>Chemical Engineering Journal</i> , 2021, 421, 127876. | 6.6 | 23 |
| 14485 | Computational Methods in Heterogeneous Catalysis. <i>Chemical Reviews</i> , 2021, 121, 1007-1048. | 23.0 | 198 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14486 | Electronic relaxation of aqueous aminoazobenzenes studied by time-resolved photoelectron spectroscopy and surface hopping TDDFT dynamics calculations. <i>Faraday Discussions</i> , 2021, 228, 226-241. | 1.6 | 6 |
| 14487 | Unraveling a trifecta of weak non-covalent interactions: The dissociation energy of the anisole-ammonia 1:1 complex. <i>Chemical Physics Letters</i> , 2021, 762, 138106. | 1.2 | 1 |
| 14488 | Equilibrium and kinetic isotopic fractionation in the CO ₂ hydration and hydroxylation reactions: Analysis of the role of hydrogen-bonding via quantum mechanical calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 292, 37-63. | 1.6 | 9 |
| 14489 | Five lead(II) coordinated polymers assembled from asymmetric azoles carboxylate ligands: Synthesis, structures and fluorescence properties. <i>Inorganica Chimica Acta</i> , 2021, 514, 120035. | 1.2 | 6 |
| 14490 | Reduktion und Umlagerung eines Bor(I)-Carbonylkomplexes. <i>Angewandte Chemie</i> , 2021, 133, 3000-3005. | 1.6 | 6 |
| 14491 | Isomerization of <i>trans</i> - ϵ -methylglutaconic acid. <i>JIMD Reports</i> , 2021, 58, 61-69. | 0.7 | 5 |
| 14492 | Decomposition Pathways of Ammonium Dinitramide (ADN) and its HNO ₃ Clusters Elucidated by DFT Calculations. <i>Propellants, Explosives, Pyrotechnics</i> , 2021, 46, 233-244. | 1.0 | 3 |
| 14493 | Comprehensive Benchmark Study on the Calculation of ²⁹ Si NMR Chemical Shifts. <i>Inorganic Chemistry</i> , 2021, 60, 272-285. | 1.9 | 14 |
| 14494 | Two-photon uncaging of bioactive thiols in live cells at wavelengths above 800 nm. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 2213-2223. | 1.5 | 7 |
| 14495 | Impact of molecular and packing structure on the charge-transport properties of hetero[8]circulenes. <i>Journal of Materials Chemistry C</i> , 2021, 9, 1451-1466. | 2.7 | 11 |
| 14496 | Insertion of Metal-Substituted Silylene into Naphthalene's Aromatic Ring and Subsequent Rearrangement for Silaspiro-Benzocycloheptenyl and Cyclobutenosilaindan Derivatives. <i>Angewandte Chemie</i> , 2021, 133, 3226-3232. | 1.6 | 4 |
| 14497 | Effect of formaldehyde properties on SnO ₂ clusters gas sensitivity: A DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 102, 107791. | 1.3 | 23 |
| 14498 | Insertion of Metal-Substituted Silylene into Naphthalene's Aromatic Ring and Subsequent Rearrangement for Silaspiro-Benzocycloheptenyl and Cyclobutenosilaindan Derivatives. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 3189-3195. | 7.2 | 15 |
| 14499 | De novo generation of optically active small organic molecules using Monte Carlo tree search combined with recurrent neural network. <i>Journal of Computational Chemistry</i> , 2021, 42, 136-143. | 1.5 | 8 |
| 14500 | Anatomy of Base Pairing in DNA by Interacting Quantum Atoms. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 211-222. | 2.5 | 9 |
| 14501 | Planar Tetracoordinate Silicon in Organic Molecules As Carbenoid-Type Amphoteric Centers: A Computational Study. <i>Chemistry - A European Journal</i> , 2021, 27, 1402-1409. | 1.7 | 10 |
| 14502 | Can density functional theory \sim Cope TM with highly fluxional shapeshifting molecules?. <i>Chemical Physics</i> , 2021, 540, 111013. | 0.9 | 15 |
| 14503 | The ¹ H and ¹³ C chemical shifts of ⁵ lignin model dimers: An evaluation of DFT functionals. <i>Journal of Molecular Structure</i> , 2021, 1226, 129300. | 1.8 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14504 | Machine learning-based prediction of enzyme substrate scope: Application to bacterial nitrilases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 336-347. | 1.5 | 30 |
| 14505 | Theoretical insights into sensing performances of rhodamine-contained two-photon fluorescent probes for mercury ion. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26435. | 1.0 | 5 |
| 14506 | Exploring the Reaction Paths on the Potential Energy Surfaces of the $S_{1,0}$ and $T_{1,0}$ States in Methylenecyclopropane. <i>Photochemistry and Photobiology</i> , 2021, 97, 126-135. | 1.3 | 2 |
| 14507 | An electrochemically controlled release of NHCs using iron bis(dithiolene) N-heterocyclic carbene complexes. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 59-71. | 3.0 | 4 |
| 14508 | Zinc oxide-quercetin nanocomposite as a smart nano-drug delivery system: Molecular-level interaction studies. <i>Applied Surface Science</i> , 2021, 536, 147741. | 3.1 | 76 |
| 14509 | Efficient hydro-finishing of polyalphaolefin based lubricants under mild reaction condition using Pd on ligands decorated halloysite. <i>Journal of Colloid and Interface Science</i> , 2021, 581, 939-953. | 5.0 | 56 |
| 14510 | Non-Planar Structures of Sterically Overcrowded Trialkylamines. <i>Chemistry - A European Journal</i> , 2021, 27, 3700-3707. | 1.7 | 3 |
| 14511 | Assessment and development of DFT with the expanded $CUAGAU$ set of group-1 cluster systems. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26453. | 1.0 | 22 |
| 14512 | Determination of theoretical calculations by DFT method and investigation of antioxidant, antimicrobial properties of olive leaf extracts from different regions. <i>Journal of Food Science and Technology</i> , 2021, 58, 1909-1917. | 1.4 | 11 |
| 14513 | Applications of isodesmic-type reactions for computational thermochemistry. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1501. | 6.2 | 25 |
| 14514 | COMPASS III: automated fitting workflows and extension to ionic liquids. <i>Molecular Simulation</i> , 2021, 47, 540-551. | 0.9 | 80 |
| 14515 | Monodentate AlEgen Anchored on Metal-Organic Framework for Fast Fluorescence Sensing of Phosphate. <i>Chinese Journal of Chemistry</i> , 2021, 39, 99-105. | 2.6 | 21 |
| 14516 | Proton-controlled non-exponential photoluminescence in a pyridylamidine-substituted Re complex. <i>Dalton Transactions</i> , 2021, 50, 7265-7276. | 1.6 | 1 |
| 14517 | Time-Dependent Density Functional Theory Study of Copper(II) Oxo Active Sites for Methane-to-Methanol Conversion in Zeolites. <i>Inorganic Chemistry</i> , 2021, 60, 1149-1159. | 1.9 | 10 |
| 14518 | Regioisomeric BODIPY derivatives: second-order nonlinear optical properties under an external electric field. <i>New Journal of Chemistry</i> , 2021, 45, 4335-4339. | 1.4 | 1 |
| 14519 | Electronic structure of solids and molecules. <i>Interface Science and Technology</i> , 2021, , 325-373. | 1.6 | 2 |
| 14520 | Mechanistic insights into the C-H activation of methane mediated by the unsupported and silica-supported VO_2OH and $CrOOH$: a DFT study. <i>RSC Advances</i> , 2021, 11, 11295-11303. | 1.7 | 3 |
| 14521 | The reversible inter-conversion of copper(II) dimers bearing phenolate-based ligands in their monomers: theoretical and experimental viewpoints. <i>New Journal of Chemistry</i> , 2021, 45, 1203-1215. | 1.4 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14522 | Synthetic- and DFT modelling studies on regioselective modified Mannich reactions of hydroxy-KYNA derivatives. <i>RSC Advances</i> , 2021, 11, 543-554. | 1.7 | 6 |
| 14523 | Ln(<i>iii</i>) complexes with a chiral 1 <i>H</i> -pyrazolo[3,4- <i>b</i>]pyridine derivative fused with a ($\hat{\alpha}$)- \pm -pinene moiety: synthesis, crystal structure, and photophysical studies in solution and in the solid state. <i>New Journal of Chemistry</i> , 2021, 45, 2276-2284. | 1.4 | 5 |
| 14524 | Color-tunable bioluminescence imaging portfolio for cell imaging. <i>Scientific Reports</i> , 2021, 11, 2219. | 1.6 | 15 |
| 14525 | Discrete unusual mixed-bridged trinuclear Coll ₂ Coll and pentanuclear NiII coordination complexes supported by a phenolate-based ligand: theoretical and experimental magneto-structural study. <i>New Journal of Chemistry</i> , 2021, 45, 6053-6066. | 1.4 | 4 |
| 14526 | Polythiophene derivatives as chemical sensors: a DFT study on the influence of side groups. <i>Journal of Molecular Modeling</i> , 2021, 27, 17. | 0.8 | 11 |
| 14527 | 3-Methyl-1,2,3-triazolium-1 <i>N</i> -dinitromethylide and the strategy of zwitterionic dinitromethyl groups in energetic materials design. <i>RSC Advances</i> , 2021, 11, 17710-17714. | 1.7 | 3 |
| 14528 | Global double hybrids do not work for charge transfer: A comment on "Double hybrids and time-dependent density functional theory: An implementation and benchmark on charge transfer excited states". <i>Journal of Computational Chemistry</i> , 2021, 42, 528-533. | 1.5 | 15 |
| 14529 | Fast estimation of the internal conversion rate constant in photophysical applications. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6344-6348. | 1.3 | 16 |
| 14530 | The effect of particle size on the optical and electronic properties of magnesium oxide nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21579-21590. | 1.3 | 3 |
| 14531 | DABCO cadmium(II) tetrakis(4-methoxyphenyl)porphyrin complex " Structure, photophysical properties, and adsorption removal of methylene blue dye. <i>Inorganica Chimica Acta</i> , 2021, 515, 120046. | 1.2 | 15 |
| 14532 | Oxidation of Pd(<i>ii</i>) with disilane in a palladium-catalyzed disilylation of aryl halides: a theoretical view. <i>Dalton Transactions</i> , 2021, 50, 7656-7666. | 1.6 | 6 |
| 14533 | Copper(<i>i</i>) and silver(<i>i</i>) chemistry of vinyltrifluoroborate supported by a bis(pyrazolyl)methane ligand. <i>Dalton Transactions</i> , 2021, 50, 7621-7632. | 1.6 | 2 |
| 14534 | Highly twisted carbazole-borane derivatives: "N stereodynamic analysis and consequences on their emission properties. <i>Organic Chemistry Frontiers</i> , 2021, 8, 4496-4507. | 2.3 | 4 |
| 14535 | Chemical structure stabilities of a Si _x F _y (<i>x</i> = 6, <i>y</i> = 12) series. <i>RSC Advances</i> , 2021, 11, 21832-21839. | 1.7 | 4 |
| 14536 | Iron- and zinc-mediated reductive coupling of styrenes and alkyl bromides: mechanistic investigation using DFT calculations. <i>Organic Chemistry Frontiers</i> , 2021, 8, 3372-3380. | 2.3 | 1 |
| 14537 | Synthesis, characterization, photophysical properties, and computational studies on N-hexylphenothiazine/cyanopyridine based π -conjugated copolymers. <i>High Performance Polymers</i> , 2021, 33, 712-726. | 0.8 | 1 |
| 14538 | A Theoretical Study of Product Selectivity in Rhodium Catalyzed Oxidative Coupling Reaction Caused by the Solvation Effect. <i>Heterocycles</i> , 2021, 103, 952. | 0.4 | 0 |
| 14539 | New Isomalabaricane-Derived Metabolites from a <i>Stelletta</i> sp. Marine Sponge. <i>Molecules</i> , 2021, 26, 678. | 1.7 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 14540 | Methyl sydnone imine and its energetic salts. <i>New Journal of Chemistry</i> , 2021, 45, 2228-2236. | 1.4 | 6 |
| 14541 | A Computational Study on the Attack of Nitrogen and Oxygen Atoms to Toluene. <i>Lecture Notes in Computer Science</i> , 2021, , 620-631. | 1.0 | 6 |
| 14542 | Approach to Increase the Utilization of Active Material in a High Sulfur-Loaded Cathode for High Areal Capacity Room-Temperature Sodium-Sulfur Batteries. <i>ACS Applied Energy Materials</i> , 2021, 4, 384-393. | 2.5 | 11 |
| 14543 | Predicting the new carbon nanocages, fullerenes: a DFT study. <i>Scientific Reports</i> , 2021, 11, 2511. | 1.6 | 12 |
| 14544 | Dissociation of dinitrogen on iron clusters: a detailed study of the Fe ₁₆ + N ₂ case. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2166-2178. | 1.3 | 6 |
| 14545 | Electrochemical reduction of CO ₂ to CO and HCOO ⁻ using metal-cyclam complex catalysts: predicting selectivity and limiting potential from DFT. <i>Dalton Transactions</i> , 2021, 50, 11446-11457. | 1.6 | 3 |
| 14546 | Acetylene-linked conjugated polymers for sacrificial photocatalytic hydrogen evolution from water. <i>Journal of Materials Chemistry A</i> , 2021, 9, 17242-17248. | 5.2 | 18 |
| 14547 | The role of dinuclearity in promoting thermally activated delayed fluorescence (TADF) in cyclometallated, N ^C N-coordinated platinum(II) complexes. <i>Journal of Materials Chemistry C</i> , 2021, 9, 10276-10287. | 2.7 | 26 |
| 14548 | A Machine Learning Approach for MP2 Correlation Energies and Its Application to Organic Compounds. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 777-790. | 2.3 | 10 |
| 14549 | Synthesis and coordination behaviour of aluminate-based quinolyl ligands. <i>Dalton Transactions</i> , 2021, 50, 14551-14559. | 1.6 | 3 |
| 14550 | Ground- and excited-state characteristics in photovoltaic polymer N2200. <i>RSC Advances</i> , 2021, 11, 20191-20199. | 1.7 | 15 |
| 14551 | Ultrahigh-yield on-surface synthesis and assembly of circumcoronene into a chiral electronic Kagome-honeycomb lattice. <i>Science Advances</i> , 2021, 7, . | 4.7 | 43 |
| 14552 | Polyeutectic-based stable and effective electrolytes for high-performance energy storage systems. <i>Energy and Environmental Science</i> , 2021, 14, 931-939. | 15.6 | 21 |
| 14553 | Equivalent Loading of Directed Arenes in Pd(II)-Catalyzed Oxidative Cross-Coupling of Aryl C-H Bonds at Room Temperature. <i>Journal of Organic Chemistry</i> , 2021, 86, 2714-2733. | 1.7 | 7 |
| 14554 | Probing Fundamental Symmetries of Deformed Nuclei in Symmetric Top Molecules. <i>Physical Review Letters</i> , 2021, 126, 023003. | 2.9 | 33 |
| 14555 | Enantioselective C-H Amination Catalyzed by Nickel Iminyl Complexes Supported by Anionic Bisoxazoline (BOX) Ligands. <i>Journal of the American Chemical Society</i> , 2021, 143, 817-829. | 6.6 | 52 |
| 14556 | Revealing structural peculiarities of homopurine GA repetition stuck by i-motif clip. <i>Nucleic Acids Research</i> , 2021, 49, 11425-11437. | 6.5 | 3 |
| 14557 | Excitation energies through Becke's exciton model within a Cartesian-grid KS DFT. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1. | 0.5 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14558 | Electron-induced fragmentation mechanisms in organic monomers and their implications for photoresist optimization for EUV lithography. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9228-9234. | 1.3 | 5 |
| 14559 | Excited state character of Cibalackrot-type compounds interpreted in terms of Hückel-aromaticity: a rationale for singlet fission chromophore design. <i>Chemical Science</i> , 2021, 12, 6159-6171. | 3.7 | 30 |
| 14560 | A combined experimental and computational investigation of the binary mixtures of 2-methylcyclohexanol and isobutanol. <i>Structural Chemistry</i> , 2021, 32, 1459-1472. | 1.0 | 0 |
| 14561 | Seven-Coordinate Tb ³⁺ Complexes with 90% Quantum Yields: High-Performance Examples of Combined Singlet- and Triplet-to-Tb ³⁺ Energy-Transfer Pathways. <i>Inorganic Chemistry</i> , 2021, 60, 892-907. | 1.9 | 33 |
| 14562 | Incorporation of tetracarboxylate ions into octacalcium phosphate for the development of next-generation biofriendly materials. <i>Communications Chemistry</i> , 2021, 4, . | 2.0 | 19 |
| 14563 | Formation of Catalytically Active Nanoparticles Under Thermolysis of Silver Chloroplatinate(II) and Chloroplatinate(IV). <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 0 |
| 14564 | Linker Expansion and Its Impact on Switchability in Pillared-Layer MOFs. <i>Inorganic Chemistry</i> , 2021, 60, 1726-1737. | 1.9 | 8 |
| 14565 | Quantitative analysis of liquid-phase adsorption over chromium-containing metal-organic frameworks of MTN topology. <i>Adsorption</i> , 2021, 27, 953-962. | 1.4 | 0 |
| 14566 | A computational study for the reaction mechanism of metal-free cyanomethylation of aryl alkynoates with acetonitrile. <i>RSC Advances</i> , 2021, 11, 18246-18251. | 1.7 | 1 |
| 14567 | Method Optimisation in Hydrophilic-Interaction Liquid Chromatography by Design of Experiments Combined with Quantitative Structure-Retention Relationships. <i>Australian Journal of Chemistry</i> , 2021, 74, 778-786. | 0.5 | 4 |
| 14568 | Synthesis of both enantiomers of lycoperdic acid, an unusual mushroom-derived amino acid. <i>Bioscience, Biotechnology and Biochemistry</i> , 2021, 85, 154-159. | 0.6 | 2 |
| 14569 | Competition between cyclization and unusual Norrish type I and type II nitro-acyl migration pathways in the photouncaging of 1-acyl-7-nitroindoline revealed by computations. <i>Scientific Reports</i> , 2021, 11, 1396. | 1.6 | 4 |
| 14570 | Synthesis, TDDFT Calculations and Biological Evaluation of Dicationic Porphyrins as Groove Binders and Antimicrobial Agents. <i>ChemistrySelect</i> , 2021, 6, 396-409. | 0.7 | 1 |
| 14571 | Revising the formation and electronic properties in flavylum derivatives. A theoretical tandem towards optimized DSSCs. <i>New Journal of Chemistry</i> , 2021, 45, 4453-4463. | 1.4 | 1 |
| 14572 | Studies on chemoselective synthesis of 1,4- and 1,2-dihydropyridine derivatives by a Hantzsch-like reaction: a combined experimental and DFT study. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 3882-3892. | 1.5 | 6 |
| 14573 | N-Doping improves charge transport and morphology in the organic non-fullerene acceptor O-IDTBR. <i>Journal of Materials Chemistry C</i> , 2021, 9, 4486-4495. | 2.7 | 17 |
| 14574 | QUANTUM CHEMICAL STUDY OF THE STABILITY OF COPPER-PALLADIUM COMPLEXES IN THE GAS PHASE. <i>Journal of Structural Chemistry</i> , 2021, 62, 9-18. | 0.3 | 2 |
| 14575 | Delocalized relativistic effects, from the viewpoint of halogen bonding. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4064-4074. | 1.3 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14576 | Mechanistic understanding of the Cu(i)-catalyzed domino reaction constructing 1-aryl-1,2,3-triazole from electron-rich aryl bromide, alkyne, and sodium azide: a DFT study. <i>Catalysis Science and Technology</i> , 2021, 11, 3208-3216. | 2.1 | 3 |
| 14577 | Influence of ligand composition on crystal structure formation – isostructurality and morphotropism. <i>CrystEngComm</i> , 2021, 23, 317-323. | 1.3 | 6 |
| 14578 | Benzobisthiadiazole-based high-spin donor-acceptor conjugated polymers with localized spin distribution. <i>Materials Advances</i> , 2021, 2, 2943-2955. | 2.6 | 10 |
| 14579 | A new perspective for evaluating the photoelectric performance of organic-inorganic hybrid perovskites based on the DFT calculations of excited states. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 11548-11556. | 1.3 | 23 |
| 14580 | Rapid detection strategies for the ultra-level chemosensing of uranyl ions. <i>Dalton Transactions</i> , 2021, 50, 14706-14713. | 1.6 | 4 |
| 14581 | A Quantum Chemistry View on Two Archetypical Paramagnetic Pentacoordinate Nickel(II) Complexes Offers a Fresh Look on Their NMR Spectra. <i>Inorganic Chemistry</i> , 2021, 60, 2068-2075. | 1.9 | 18 |
| 14582 | Evaluation of nine condensed-phase force fields of the GROMOS, CHARMM, OPLS, AMBER, and OpenFF families against experimental cross-solvation free energies. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13055-13074. | 1.3 | 9 |
| 14583 | Understanding the reaction mechanism of gold-catalyzed reactions of 2,1-benzisoxazoles with propiolates and ynamides. <i>Organic Chemistry Frontiers</i> , 2021, 8, 3342-3353. | 2.3 | 3 |
| 14584 | Identification of beryllium fluoride complexes in mechanically distorted gels using quadrupolar split ⁹ Be NMR spectra resolved with solution-state selective cross-polarization. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16932-16941. | 1.3 | 1 |
| 14585 | Electronic Structure of Paramagnetic Iron and Manganese Cluster Compounds: Historical Developments and Current Understanding. , 2021, , 45-81. | | 0 |
| 14586 | Assessing the Applicability of the Geometric Counterpoise Correction in B2PLYP/Double- η Calculations for Thermochemistry, Kinetics, and Noncovalent Interactions*. <i>Australian Journal of Chemistry</i> , 2021, , . | 0.5 | 2 |
| 14587 | A new computational strategy to calculate the surface energy of a dipolar crystal surface. <i>CrystEngComm</i> , 2021, 23, 4791-4798. | 1.3 | 2 |
| 14588 | Preparation and characterization of a copper oxide nanoparticle-supported red-mud catalyst for liquid phase oxidation of ethyl benzene to acetophenone. <i>New Journal of Chemistry</i> , 2021, 45, 13070-13079. | 1.4 | 7 |
| 14589 | Calculated oxidation potentials predict reactivity in Baeyer-Mills reactions. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 7575-7580. | 1.5 | 8 |
| 14590 | Valence-shell photoelectron circular dichroism of ruthenium(ⁱⁱⁱ)-tris-(acetylacetonato) gas-phase enantiomers. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24140-24153. | 1.3 | 6 |
| 14591 | DFT insights into the Ni-catalyzed regioselective hydrocarboxylation of unsaturated alkenes with CO ₂ . <i>Dalton Transactions</i> , 2021, 50, 15084-15093. | 1.6 | 4 |
| 14592 | Dimeric Mn(ii), Co(ii), Ni(ii) and Cu(ii) complexes of a common carboxylate-appended (2-pyridyl)alkylamine ligand: structure, magnetism and DFT study. <i>New Journal of Chemistry</i> , 2021, 45, 16019-16029. | 1.4 | 10 |
| 14593 | Unravelling the structures of sodiated β -cyclodextrin and its fragments. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13714-13723. | 1.3 | 15 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 14594 | An oxidant- and catalyst-free electrooxidative cross-coupling approach to 3-tetrahydroisoquinoline substituted coumarins. <i>Green Chemistry</i> , 2021, 23, 1274-1279. | 4.6 | 15 |
| 14595 | Heavy-element π -ligand covalence: ligand noninnocence in molybdenum and tungsten Viking-helmet Corroles. <i>Dalton Transactions</i> , 2021, 50, 12843-12849. | 1.6 | 6 |
| 14596 | Synthesis and Electronic Properties of Diketopyrrolopyrrole-Based Polymers with and without Ring-Fusion. <i>Macromolecules</i> , 2021, 54, 970-980. | 2.2 | 23 |
| 14598 | The $[Ag_{25}Cu_4H_8Br_6(CPh)_3(PPh_3)_2]_3$ silver hydride core protected by $[CuAg_3(CPh)_3(PPh_3)_3]^+$ motifs. <i>Dalton Transactions</i> , 2021, 50, 5659-5665. | 1.6 | 11 |
| 14599 | Exploring vibronic coupling in the benzene radical cation and anion with different levels of the GW approximation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19054-19070. | 1.3 | 1 |
| 14600 | Achieving full-color emission of Cu nanocluster self-assembly nanosheets by the virtue of halogen effects. <i>Soft Matter</i> , 2021, 17, 4550-4558. | 1.2 | 5 |
| 14601 | Unveiling the complex pattern of intermolecular interactions responsible for the stability of the DNA duplex. <i>Chemical Science</i> , 2021, 12, 12785-12793. | 3.7 | 11 |
| 14602 | Structure, Electronic, and Charge Transfer Properties of Organic Photovoltaics from Density Functional Theory Methods. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2021, , 57-79. | 0.6 | 0 |
| 14603 | Prediction of Heats of Formation of Polycyclic Saturated Hydrocarbons Using the XYG3 Double Hybrid Functionals. <i>Springer Series in Materials Science</i> , 2021, , 245-255. | 0.4 | 1 |
| 14604 | Activation of hydrogen peroxide by the nitrate anion in micellar media. <i>Green Chemistry</i> , 2021, 23, 1965-1971. | 4.6 | 3 |
| 14605 | Carboxylic acids as anchoring components on aluminum oxide for the alignment relay technique of single-walled carbon nanotubes. <i>New Journal of Chemistry</i> , 2021, 45, 5340-5349. | 1.4 | 4 |
| 14606 | EPR-derived structures of flavin radical and iron-sulfur clusters from <i>Methylosinus sporium</i> 5 reductase. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 1279-1289. | 3.0 | 5 |
| 14607 | Anomeric effect, hyperconjugation and electrostatics: lessons from complexity in a classic stereoelectronic phenomenon. <i>Chemical Society Reviews</i> , 2021, 50, 10212-10252. | 18.7 | 78 |
| 14608 | Structures and hydrogen bonding of 1,7-dioxaspiro[5.5]undecane and its hydrates. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19289-19296. | 1.3 | 1 |
| 14609 | Reduced-dimensional surface hopping with offline-online computations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19547-19557. | 1.3 | 2 |
| 14610 | Redesigning donor-acceptor Stenhouse adduct photoswitches through a joint experimental and computational study. <i>Chemical Science</i> , 2021, 12, 2916-2924. | 3.7 | 18 |
| 14611 | Nanostructured Palladacycle and its Decorated Ag-NP Composite: Synthesis, Morphological Aspects, Characterization, Quantum Chemical Calculation and Antimicrobial Activity. <i>Arabian Journal for Science and Engineering</i> , 2021, 46, 5655-5669. | 1.7 | 2 |
| 14612 | Acenes and phenacenes in their lowest-lying triplet states. Does kinked remain more stable than straight?. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13574-13582. | 1.3 | 18 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14613 | Unravelling the nature of a toluene–fumarionitrile complex. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16128-16141. | 1.3 | 2 |
| 14614 | Highly-efficient production of spherical co-agglomerates of drugs via an organic solvent-free process and a mechanism study. <i>Green Chemistry</i> , 2021, 23, 2710-2721. | 4.6 | 22 |
| 14615 | Biochemical and crystallographic investigations into isonitrile formation by a nonheme iron-dependent oxidase/decarboxylase. <i>Journal of Biological Chemistry</i> , 2021, 296, 100231. | 1.6 | 16 |
| 14616 | Electronic structure and transport properties of coupled CdS/ZnSe quantum dots. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 125002. | 0.7 | 3 |
| 14617 | Origins of Optical Activity in an Oxo-Helicene: Experimental and Computational Studies. <i>ACS Omega</i> , 2021, 6, 2420-2428. | 1.6 | 18 |
| 14618 | Quantum Algorithm for Simulating Single-Molecule Electron Transport. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 1256-1261. | 2.1 | 6 |
| 14619 | Gaseous cyclodextrin-cyclododecaborate complexes $\beta\text{-CD} \cdot \text{B}_{12}\text{X}_{12}$ ($\beta = \beta^1, \beta^2, \text{ and } \beta^3$; X = F, Cl, Br, and I): electronic structures and intramolecular interactions. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13447-13457. | 1.3 | 8 |
| 14620 | Coordination-induced emission enhancement in copper(I) iodide coordination polymers supported by 2-(alkylsulfanyl)pyrimidines. <i>Dalton Transactions</i> , 2021, 50, 9317-9330. | 1.6 | 17 |
| 14621 | Revealing the electronic properties of the B–B bond: the bis-catecholato diboron molecule. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 23517-23525. | 1.3 | 2 |
| 14622 | Biological halogen bonds in protein–ligand complexes: a combined QTAIM and NCIPLOT study in four representative cases. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 6858-6864. | 1.5 | 10 |
| 14623 | Photoactive Pt(II) and Pd(II) complexes of <i>N,N</i> -diethyl- <i>N</i> - ϵ -(2,3,4,5-trimethoxybenzoyl)thiourea: synthesis, crystal structures, DFT and cytotoxicity studies. <i>New Journal of Chemistry</i> , 2021, 45, 14703-14712. | 1.4 | 3 |
| 14624 | Structures of the archaerhodopsin-3 transporter reveal that disordering of internal water networks underpins receptor sensitization. <i>Nature Communications</i> , 2021, 12, 629. | 5.8 | 22 |
| 14625 | Hydrogen evolution by polymer photocatalysts; a possible photocatalytic cycle. <i>Sustainable Energy and Fuels</i> , 2021, 5, 2622-2632. | 2.5 | 10 |
| 14626 | On the anomeric preference of the isothiocyanato group. <i>New Journal of Chemistry</i> , 2021, 45, 14111-14125. | 1.4 | 1 |
| 14627 | Rhodium(bisoxazolinephosphine)-catalyzed regio- and enantioselective amination of allylic carbonates: a computational study. <i>Organic Chemistry Frontiers</i> , 2021, 8, 3320-3331. | 2.3 | 7 |
| 14628 | Ni pincer complex catalytic hydroboration of CO_2 : a DFT study on the influence of borane reductants on selective reduction. <i>New Journal of Chemistry</i> , 2021, 45, 11275-11283. | 1.4 | 4 |
| 14629 | Phenanthroimidazole derivatives showing mild intramolecular charge transfer and high quantum yields and their applications in OLEDs. <i>New Journal of Chemistry</i> , 2021, 45, 16238-16247. | 1.4 | 12 |
| 14630 | Density Sensitivity of Empirical Functionals. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 800-807. | 2.1 | 29 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14631 | Re-examining the electronic structure of fluorescent tetra-silver clusters in zeolites. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1984-1993. | 1.3 | 6 |
| 14632 | Luminescent Cu ₄ I ₄ -cubane clusters based on <i>N</i> -methyl-5,10-dihydrophenarsazines. <i>Dalton Transactions</i> , 2021, 50, 13421-13429. | 1.6 | 13 |
| 14633 | Hydrogenation of Cyclic 1,3-Diones to Their 1,3-Diols Using Heterogeneous Catalysts: Toward a Facile, Robust, Scalable, and Potentially Bio-Based Route. <i>ACS Omega</i> , 2021, 6, 4313-4328. | 1.6 | 4 |
| 14634 | Synthesis and Characterization of the Energetic 3-Azido-5-amino-6-nitro-1,2,4-triazine. <i>Propellants, Explosives, Pyrotechnics</i> , 2021, 46, 214-221. | 1.0 | 11 |
| 14635 | Quantum-Chemical Simulation of the Adsorption of OH ⁻ Ions on Au(111). <i>Russian Journal of Electrochemistry</i> , 2021, 57, 22-29. | 0.3 | 0 |
| 14636 | The structural manipulation of a series of Ni ₄ defective dicubanes: Synthesis, X-ray Structures, Magnetic and Computational analyses. <i>Dalton Transactions</i> , 2021, 50, 5318-5326. | 1.6 | 5 |
| 14637 | Simulating fullerene polyhedral formation from planar precursors. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6561-6573. | 1.3 | 0 |
| 14638 | Single-molecule imaging and kinetic analysis of intermolecular polyoxometalate reactions. <i>Chemical Science</i> , 2021, 12, 7377-7387. | 3.7 | 18 |
| 14639 | The importance of finite temperature and vibrational sampling in the absorption spectrum of a nitro-functionalized Ru(^{II}) water oxidation catalyst. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17724-17733. | 1.3 | 2 |
| 14640 | Theoretical study of rhodium- and cobalt-catalyzed decarboxylative transformations of isoxazolones: origin of product selectivity. <i>Organic Chemistry Frontiers</i> , 2021, 8, 1257-1266. | 2.3 | 2 |
| 14641 | Structural and electronic properties of TiO ₂ from first principles calculations. , 2021, , 67-85. | | 2 |
| 14642 | Transition-metal-mediated reduction and reversible double-cyclization of cyanuric triazide to an asymmetric bitetrazolate involving cleavage of the six-membered aromatic ring. <i>Chemical Science</i> , 2021, 12, 2268-2275. | 3.7 | 3 |
| 14643 | A ⁿ fusion strategy to design bipolar organic materials for high-energy-density symmetric batteries. <i>Journal of Materials Chemistry A</i> , 2021, 9, 14485-14494. | 5.2 | 30 |
| 14644 | Coordination Geometrical Effect on Ligand-to-Metal Charge Transfer-Dependent Energy Transfer Processes of Luminescent Eu(III) Complexes. <i>Journal of Physical Chemistry A</i> , 2021, 125, 209-217. | 1.1 | 21 |
| 14645 | The Role of Range-Separated Correlation in Long-Range Corrected Hybrid Functionals. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 1207-1213. | 2.1 | 7 |
| 14646 | Donor acceptor fluorophores: synthesis, optical properties, TD-DFT and cytotoxicity studies. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 1835-1846. | 1.5 | 12 |
| 14647 | Highly efficient visible-light photocatalytic ethane oxidation into ethyl hydroperoxide as a radical reservoir. <i>Chemical Science</i> , 2021, 12, 5825-5833. | 3.7 | 12 |
| 14648 | Understanding polyoxometalates as water oxidation catalysts through iron <i>vs.</i> cobalt reactivity. <i>Chemical Science</i> , 2021, 12, 8755-8766. | 3.7 | 23 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 14649 | Efficient and low-scaling linear-response time-dependent density functional theory implementation for core-level spectroscopy of large and periodic systems. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4736-4746. | 1.3 | 14 |
| 14650 | Commentary toward the 20th Anniversary of the Society of Computer Chemistry, Japan. <i>Journal of Computer Chemistry Japan</i> , 2021, 20, A26-A40. | 0.0 | 0 |
| 14651 | Computational approaches to dissociative chemisorption on metals: towards chemical accuracy. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8962-9048. | 1.3 | 47 |
| 14652 | Quantitative Comparison of Experimental and Computed IR-Spectra Extracted from Ab Initio Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 985-995. | 2.3 | 9 |
| 14653 | Anion photoelectron spectroscopy and quantum chemistry calculations of TaSi ₁₆ clusters: global minimum fullerene-like cage structure, bonding and superatom properties. <i>New Journal of Chemistry</i> , 2021, 45, 5266-5271. | 1.4 | 5 |
| 14654 | High-Resolution Rotational Spectroscopy and Interstellar Search for Isopropyl Isothiocyanate. <i>ACS Earth and Space Chemistry</i> , 2021, 5, 33-39. | 1.2 | 4 |
| 14655 | Peptide Hydrolysis by Metal (Oxa)cyclen Complexes: Revisiting the Mechanism and Assessing Ligand Effects. <i>Inorganic Chemistry</i> , 2021, 60, 807-815. | 1.9 | 5 |
| 14656 | Mechanism of nickel-catalyzed direct carbonyl-Heck coupling reaction: the crucial role of second-sphere interactions. <i>Dalton Transactions</i> , 2021, 50, 2654-2662. | 1.6 | 10 |
| 14657 | Insights into the structure and ionic transport in water-in-bisalt™ electrolytes for lithium-ion batteries. <i>Materials Advances</i> , 2021, 2, 7691-7700. | 2.6 | 4 |
| 14658 | Stabilities, Electronic Structures, and Bonding Properties of 20-Electron Transition Metal Complexes (Cp) ₂ TMO and their One-Dimensional Sandwich Molecular Wires (Cp = Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 387 125, 721-730. | 1.1 | 2 |
| 14659 | Towards a converged strategy for including microsolvation in reaction mechanism calculations. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 473-492. | 1.3 | 23 |
| 14660 | Vibrational dynamics of hydrogen molecules under intense THz waves. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, 70, 243101. | 0.2 | 0 |
| 14661 | <i>in silico</i> design to enhance the barrier height for magnetization reversal in Dy(III) sandwich complexes by stitching them under the umbrella of corannulene. <i>Chemical Science</i> , 2021, 12, 11506-11514. | 3.7 | 7 |
| 14662 | Charge Transfer Excitation and Asymmetric Energy Transfer at the Interface of Pentacene-Perfluoropentacene Heterostacks. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 5284-5292. | 4.0 | 5 |
| 14663 | A Computational Analysis of the Reaction of Atomic Oxygen O(³ P) with Acrylonitrile. <i>Lecture Notes in Computer Science</i> , 2021, , 339-350. | 1.0 | 0 |
| 14664 | Replacing hybrid density functional theory: motivation and recent advances. <i>Chemical Society Reviews</i> , 2021, 50, 8470-8495. | 18.7 | 80 |
| 14665 | Intermolecular Interactions and Solubility Behavior of Multicomponent Crystal Forms of 2,4-dichlorophenoxyacetic acid: Design, Structure Analysis, and Solid-State Characterization. <i>CrystEngComm</i> , 0, , . | 1.3 | 12 |
| 14666 | Photodissociation dynamics of halogenated aromatic molecules: the case of core-ionized tetrabromothiophene. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21249-21261. | 1.3 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14685 | Computational Investigations of the Lithium Superoxide Dimer Rearrangement on Noisy Quantum Devices. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1827-1836. | 1.1 | 37 |
| 14686 | Structural and Thermodynamics Studies on Polyaminophosphonate Ligands for Uranyl Decorporation. <i>Inorganic Chemistry</i> , 2021, 60, 2149-2159. | 1.9 | 7 |
| 14687 | Assembly of [Ni(Schiff)] Films on an Inert Surface: A Multiscale Computational Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 2926-2937. | 1.5 | 4 |
| 14688 | Non-Covalent Interactions Atlas Benchmark Data Sets 3: Repulsive Contacts. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1548-1561. | 2.3 | 42 |
| 14689 | From Missing Links to New Records: A Series of Novel Polychlorine Anions. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 1034-1040. | 1.0 | 9 |
| 14690 | <i>Ab initio</i> electronic density in solids by many-body plane-wave auxiliary-field quantum Monte Carlo calculations. <i>Physical Review B</i> , 2021, 103, . | 1.1 | 8 |
| 14691 | Observation and laser spectroscopy of ytterbium monomethoxide, YbOCH_3 . <i>Physical Review A</i> , 2021, 103, . | 1.0 | 2 |
| 14692 | Mechanism and Origins of Stereoselectivity of the Aldol-Tishchenko Reaction of Sulfinimines. <i>Journal of Organic Chemistry</i> , 2021, 86, 4296-4303. | 1.7 | 7 |
| 14693 | Catalyzed-like water enhanced mechanism of CO ₂ conversion to methanol. <i>Arabian Journal of Chemistry</i> , 2021, 14, 102955. | 2.3 | 1 |
| 14694 | Computer-assisted catalyst development via automated modelling of conformationally complex molecules: application to diphosphinoamine ligands. <i>Scientific Reports</i> , 2021, 11, 4534. | 1.6 | 5 |
| 14696 | Dissociative Ionization of Molecular CF ₂ Br ₂ under 800 and 400 nm Intense Femtosecond Laser Fields. <i>Applied Sciences (Switzerland)</i> , 2021, 11, 1704. | 1.3 | 1 |
| 14697 | Synthesis and Characterization of Tellurium Catecholates and Their <i>N</i> -Oxide Adducts. <i>Inorganic Chemistry</i> , 2021, 60, 3460-3470. | 1.9 | 8 |
| 14698 | Optimized structure and electronic band gap of monolayer GeSe from quantum Monte Carlo methods. <i>Physical Review Materials</i> , 2021, 5, . | 0.9 | 16 |
| 14699 | Prediction of Spin Density, Baird's Antiaromaticity, and Singlet-Triplet Energy Gap in Triplet-State Polybenzenoid Systems from Simple Structural Motifs. <i>Chemistry - A European Journal</i> , 2021, 27, 6923-6935. | 1.7 | 13 |
| 14700 | Demystifying Chronic Kidney Disease of Unknown Etiology (CKDu): Computational Interaction Analysis of Pesticides and Metabolites with Vital Renal Enzymes. <i>Biomolecules</i> , 2021, 11, 261. | 1.8 | 5 |
| 14701 | Heterogeneous Intramolecular Electric Field as a Descriptor of Diels-Alder Reactivity. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1289-1298. | 1.1 | 9 |
| 14702 | Fungal Dioxygenase AsqJ Is Promiscuous and Bimodal: Substrate-Directed Formation of Quinolones versus Quinazolinones. <i>Angewandte Chemie</i> , 2021, 133, 8378-8383. | 1.6 | 2 |
| 14703 | A quantitative evaluation of computational methods to accelerate the study of alloxazine-derived electroactive compounds for energy storage. <i>Scientific Reports</i> , 2021, 11, 4089. | 1.6 | 11 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14704 | Characterization of the mechanical and structural properties of <sc>PGA</sc>/<sc>TMC</sc> copolymer for cardiac tissue engineering. <i>Microscopy Research and Technique</i> , 2021, 84, 1596-1606. | 1.2 | 8 |
| 14705 | The 2,2,4,4-tetrafluoro-1,3-dithietane- $\bar{N}H_3$ complex: A rotational study reveals a $N\bar{H}\cdots f$ -hole interaction. <i>Journal of Molecular Spectroscopy</i> , 2021, 376, 111409. | 0.4 | 2 |
| 14706 | Switching Site Reactivity in Hydrogenase Model Systems by Introducing a Pendant Amine Ligand. <i>ACS Omega</i> , 2021, 6, 4192-4203. | 1.6 | 6 |
| 14707 | Effect of varying the TD-Ic-DFTB range-separation parameter on charge and energy transfer in a model pentacene/buckminsterfullerene heterojunction. <i>Journal of Chemical Physics</i> , 2021, 154, 054102. | 1.2 | 9 |
| 14708 | Ethylene Glycol Dihedral Angle Dynamics: Relating Molecular Conformation to the Raman Spectrum of the Liquid. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1888-1895. | 1.2 | 12 |
| 14709 | Application of \hat{P}^2 -Phosphorylated Nitroethenes in [3+2] Cycloaddition Reactions Involving Benzonitrile N-Oxide in the Light of a DFT Computational Study. <i>Organics</i> , 2021, 2, 26-37. | 0.6 | 13 |
| 14710 | Insights into the Chiral Phosphoric Acid-Catalyzed Dynamic Kinetic Asymmetric Hydroamination of Racemic Allenes: An Allyl Carbocation/Phosphate Pair Mechanism. <i>Journal of Organic Chemistry</i> , 2021, 86, 4121-4130. | 1.7 | 8 |
| 14711 | High Power and Energy Density Aqueous Proton Battery Operated at $\hat{a}^\circ 90^\circ \hat{A}^\circ C$. <i>Advanced Functional Materials</i> , 2021, 31, 2010127. | 7.8 | 77 |
| 14712 | Solvents for Processing Stable Tin Halide Perovskites. <i>ACS Energy Letters</i> , 2021, 6, 959-968. | 8.8 | 76 |
| 14713 | Theoretical insight on the solvation properties of Zn^{2+} in pure liquid ammonia: A quantum mechanical molecular charges field molecular dynamics (QMCF-MD) study. <i>Journal of Molecular Liquids</i> , 2021, 324, 114737. | 2.3 | 1 |
| 14714 | L_{γ}^{\pm} Irradiation of Superhydrogenated Coronene Films: Implications for $H_{2</sub>2</sub>}$ Formation. <i>Astrophysical Journal Letters</i> , 2021, 908, L18. | 3.0 | 4 |
| 14715 | Tetranitratopalladate(II) Salts with Tetraalkylammonium Cations: Structural Aspects, Reactivity, and Applicability toward Palladium Deposition for Catalytic Applications. <i>Inorganic Chemistry</i> , 2021, 60, 2983-2995. | 1.9 | 6 |
| 14716 | Quantum-Chemical Investigation of Pb^{2+} Ion Adsorption at Au(111) from Alkaline Medium. <i>Russian Journal of Electrochemistry</i> , 2021, 57, 141-148. | 0.3 | 0 |
| 14717 | Quantum Chemical Simulation of the Q_y Absorption Spectrum of Zn Chlorin Aggregates for Artificial Photosynthesis. <i>Molecules</i> , 2021, 26, 1086. | 1.7 | 1 |
| 14718 | Describing Polytopal Rearrangement Processes of Octacoordinate Structures. I. Renewed Insights into Fluxionality of the Rhenium Polyhydride Complex $ReH_{5</sub>3</sub>}(PPh_{3</sub>3</sub>)₂(Pyridine)$. <i>Inorganic Chemistry</i> , 2021, 60, 2492-2502. | 1.9 | 6 |
| 14719 | Collision-Induced dissociation of $[UO_2(NO_3)_3]^{\hat{a}}$ and $[UO_2(NO_3)_2(O_2)]^{\hat{a}}$ and reactions of product ions with H_2O and O_2 . <i>Journal of Mass Spectrometry</i> , 2021, 56, e4705. | 0.7 | 4 |
| 14720 | A small-molecular inhibitor against <i>Proteus mirabilis</i> urease to treat catheter-associated urinary tract infections. <i>Scientific Reports</i> , 2021, 11, 3726. | 1.6 | 19 |
| 14721 | Fungal Dioxxygenase AsqJ Is Promiscuous and Bimodal: Substrate- \hat{E} Directed Formation of Quinolones versus Quinazolinones. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 8297-8302. | 7.2 | 15 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14722 | Olive-Shaped Organic Cages: Synthesis and Remarkable Promotion of Hydrazone Condensation through Encapsulation in Water. <i>Journal of Organic Chemistry</i> , 2021, 86, 3943-3951. | 1.7 | 11 |
| 14723 | Nuclear magnetic resonance parameters in Zn ₂ , Cd ₂ and Hg ₂ dimers: relativistic calculations. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1. | 0.5 | 4 |
| 14724 | Effect of Methylmercury Binding on the Peroxide-Reducing Potential of Cysteine and Selenocysteine. <i>Inorganic Chemistry</i> , 2021, 60, 4646-4656. | 1.9 | 15 |
| 14725 | Hydrogen bonding interactions in the 1,1,1,3,3,3-hexafluoro-2-propanol TM 1,4-dioxane complex: Rotational spectroscopy and density functional theory calculations. <i>Journal of Molecular Spectroscopy</i> , 2021, 376, 111408. | 0.4 | 2 |
| 14726 | Electronic structure of Schiff-base peroxo{2,2- TM [1,2-phenylenebis(nitrilomethanylylidene)]bis(6-methoxyphenolato)}titanium(IV) monohydrate: a possible model structure of the reaction center for the theoretical study of hemoglobin. <i>IUCr</i> , 2021, 8, 295-304. | 1.0 | 2 |
| 14727 | In situ simultaneous electrochemical ESR study of radicals generated from 2,2-dinitroethene-1,1-diamine (FOX-7). Intramolecular chemical exchange resulting in an alternation line-width effect. <i>Journal of Magnetic Resonance</i> , 2021, 323, 106895. | 1.2 | 0 |
| 14728 | Spatial Contributions to Nuclear Magnetic Shieldings. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1778-1786. | 1.1 | 17 |
| 14729 | Bicyclic Boronate TM Lactamase Inhibitors: The Present Hope against Deadly Bacterial Pathogens. <i>Advanced Therapeutics</i> , 2021, 4, 2000246. | 1.6 | 12 |
| 14730 | Preliminary Identification of Hamamelitannin and Rosmarinic Acid as COVID-19 Inhibitors Based on Molecular Docking. <i>Letters in Drug Design and Discovery</i> , 2021, 18, 67-75. | 0.4 | 7 |
| 14731 | Modeling Metal-Catalyzed Polyethylene Depolymerization: [(Phen)Pd(X)] ⁺ (X = H and CH ₃) Catalyze the Decomposition of Hexane into a Mixture of Alkenes via a Complex Reaction Network. <i>Organometallics</i> , 2021, 40, 857-868. | 1.1 | 7 |
| 14732 | Quantum Simulations of Hydrogen Bonding Effects in Glycerol Carbonate Electrolyte Solutions. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2157-2166. | 1.2 | 7 |
| 14733 | Understanding the Mechanistic Requirements for Efficient and Stereoselective Alkene Epoxidation by a Cytochrome P450 Enzyme. <i>ACS Catalysis</i> , 2021, 11, 1995-2010. | 5.5 | 30 |
| 14734 | Excited-state electronic properties, structural studies, noncovalent interactions, and inhibition of the novel severe acute respiratory syndrome coronavirus 2 proteins in Ripretinib by first-principle simulations. <i>Journal of Molecular Liquids</i> , 2021, 324, 115134. | 2.3 | 23 |
| 14735 | Synthesis, Structural Features and Physical Properties of a Family of Triply Bridged Dinuclear 3d-4f Complexes. <i>Magnetochemistry</i> , 2021, 7, 22. | 1.0 | 4 |
| 14736 | Functionalization of Gold Nanostars with Cationic TM -Cyclodextrin-Based Polymer for Drug Co-Loading and SERS Monitoring. <i>Pharmaceutics</i> , 2021, 13, 261. | 2.0 | 15 |
| 14737 | Benchmarking Magnetizabilities with Recent Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1457-1468. | 2.3 | 43 |
| 14738 | Spin TM Orbit Coupling Changes the Identity of the Hyper-Open-Shell Ground State of Ce ⁺ , and the Bond Dissociation Energy of CeH ⁺ Proves to Be Challenging for Theory. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1421-1434. | 2.3 | 5 |
| 14739 | Structure and Potential TM Dependent Selectivity in Redox TM Metallopolymers: Electrochemically Mediated Multicomponent Metal Separations. <i>Advanced Functional Materials</i> , 2021, 31, 2009307. | 7.8 | 30 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14740 | Chalcogen bonds: Hierarchical <i>ab initio</i> benchmark and density functional theory performance study. <i>Journal of Computational Chemistry</i> , 2021, 42, 688-698. | 1.5 | 21 |
| 14741 | Adaptive Aromaticity in Metallasilapentalynes. <i>Organometallics</i> , 2021, 40, 899-906. | 1.1 | 16 |
| 14742 | Exceptional Sodium-Ion Storage by an Aza-Covalent Organic Framework for High Energy and Power Density Sodium-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 15083-15091. | 4.0 | 67 |
| 14743 | Thermal curing mechanism of acetylene-terminated polyimides: A combination of density functional theory computation and microkinetic analysis. <i>Polymer</i> , 2021, 218, 123529. | 1.8 | 6 |
| 14744 | Computational exploration of β -lactone rearrangements and the cyclic halonium zwitterion from bromination of acrylate anion in water: Implicit vs. explicit solvation. <i>Tetrahedron</i> , 2021, 84, 131989. | 1.0 | 0 |
| 14745 | Polyradical PROXYL/TEMPO Conjugates Connected by Ester/Amide Bridges: Synthesis, Physicochemical Studies, and DFT Calculations. <i>ChemPlusChem</i> , 2021, 86, 396-405. | 1.3 | 3 |
| 14746 | New Cationic fac-[Re(CO) ₃ (deeb)B ₂] ⁺ Complex, Where B ₂ Is a Benzimidazole Derivative, as a Potential New Luminescent Dye for Proteins Separated by SDS-PAGE. <i>Frontiers in Chemistry</i> , 2021, 9, 647816. | 1.8 | 3 |
| 14747 | A systematic study of structures, stability, and electronic properties of alloy clusters AlBe ($n = 12$): Comparison with pure beryllium clusters. <i>Polyhedron</i> , 2021, 196, 115005. | 1.0 | 2 |
| 14748 | Selectivity and competition between N-H and C-H bond activation using an organoplatinum (II) complex. <i>Applied Organometallic Chemistry</i> , 2021, 35, e6234. | 1.7 | 3 |
| 14749 | Growth and Equilibrium Morphology of Hydrohalite (NaCl·2H ₂ O) and Its Epitaxy with Hexagonal Ice Crystals. <i>Journal of Physical Chemistry C</i> , 2021, 125, 6923-6932. | 1.5 | 1 |
| 14750 | Phenyl Trifluoromethane sulfonate as a novel electrolyte additive for enhancing performance of LiNi _{0.6} Co _{0.2} Mn _{0.2} O ₂ /Graphite cells working in wide temperature ranges. <i>Journal of Power Sources</i> , 2021, 487, 229416. | 4.0 | 13 |
| 14751 | When Does Fusing Two Rings Not Yield a Larger Ring? The Curious Case of BOPHY. <i>Journal of Organic Chemistry</i> , 2021, 86, 4547-4556. | 1.7 | 4 |
| 14752 | Analytical Time-Dependent Long-Range Corrected Density Functional Tight Binding (TD-LC-DFTB) Gradients in DFTB+: Implementation and Benchmark for Excited-State Geometries and Transition Energies. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2266-2282. | 2.3 | 10 |
| 14753 | Pragmatic Improvement of Magnetic Exchange Couplings from Subsystem Density-Functional Theory through Orthogonalization of Subsystem Orbitals. <i>Journal of Physical Chemistry C</i> , 2021, 125, 6176-6188. | 1.5 | 3 |
| 14754 | Chemo- and Stereoselective Polymerization of Polar Divinyl Monomers by Rare-Earth Complexes. <i>Macromolecules</i> , 2021, 54, 3181-3190. | 2.2 | 11 |
| 14755 | Reaction Mechanisms and Rate Constants of Auto-catalytic Urethane Formation and Cleavage Reactions. <i>ChemistryOpen</i> , 2021, 10, 534-544. | 0.9 | 11 |
| 14756 | Prediction of drug-carrier interactions of PLA and PLGA drug-loaded nanoparticles by molecular dynamics simulations. <i>European Polymer Journal</i> , 2021, 147, 110292. | 2.6 | 24 |
| 14757 | Systematic Design of a Frustrated Lewis Pair Containing Methyleneborane and Carbene for Dinitrogen Activation. <i>Inorganic Chemistry</i> , 2021, 60, 5598-5606. | 1.9 | 32 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14758 | Exploring the Limits of the XYG3-Type Doubly Hybrid Approximations for the Main-Group Chemistry: The xDH@B3LYP Model. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2638-2644. | 2.1 | 17 |
| 14759 | Spatial donor/acceptor architecture for intramolecular charge-transfer emitter. <i>Chinese Chemical Letters</i> , 2021, 32, 1245-1248. | 4.8 | 17 |
| 14760 | Localized electronic vacancy level and its effect on the properties of doped manganites. <i>Scientific Reports</i> , 2021, 11, 6706. | 1.6 | 8 |
| 14761 | Synthesis of (4R)-2-(3-hydroxyphenyl)thiazolidine-4-carboxylic acid substituted phthalocyanines: Anticancer activity on different cancer cell lines and molecular docking studies. <i>Applied Organometallic Chemistry</i> , 2021, 35, e6242. | 1.7 | 13 |
| 14762 | Systematic Detection and Characterization of Hydrogen Bonding in Proteins via Local Vibrational Modes. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2551-2565. | 1.2 | 15 |
| 14763 | Computational Identification of Connected MOF@COF Materials. <i>Journal of Physical Chemistry C</i> , 2021, 125, 5897-5903. | 1.5 | 12 |
| 14764 | Novel (Phenothiazinyl)Vinyl-Pyridinium Dyes and Their Potential Applications as Cellular Staining Agents. <i>International Journal of Molecular Sciences</i> , 2021, 22, 2985. | 1.8 | 4 |
| 14765 | Surface-Enhanced Raman Spectroscopy for Bisphenols Detection: Toward a Better Understanding of the Analyte-Nanosystem Interactions. <i>Nanomaterials</i> , 2021, 11, 881. | 1.9 | 14 |
| 14766 | Bioactive Tryptophan-Based Copper Complex with Auxiliary β -Carboline Spectacle Potential on Human Breast Cancer Cells: In Vitro and In Vivo Studies. <i>Molecules</i> , 2021, 26, 1606. | 1.7 | 6 |
| 14767 | B111, B112, B113, and B114: The most stable core-shell borospherenes with an icosahedral B12 core at the center exhibiting superatomic behaviors. <i>Nano Research</i> , 2021, 14, 4719-4724. | 5.8 | 16 |
| 14768 | Ir ^{III} -Pyridoannulated N-Heterocyclic Carbene Complexes: Potent Theranostic Agents via Mitochondria Targeting. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 1551-1564. | 1.0 | 3 |
| 14769 | Nonuniform Proton Transfer and Strong Hydrogen Bonding within Cation, Anion, and Neutral Clusters of Ammonia and Hydrogen Fluoride. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2546-2557. | 1.1 | 2 |
| 14770 | Reversible Addition of Carbon Dioxide to Main Group Metal Complexes at Temperatures about 0 °C. <i>Chemistry - A European Journal</i> , 2021, 27, 5745-5753. | 1.7 | 22 |
| 14771 | Confinement of the antitumoral drug cisplatin inside edge-functionalized carbon nanotubes and its release near lipid membrane. <i>European Physical Journal D</i> , 2021, 75, 1. | 0.6 | 4 |
| 14772 | How the replacement of cholesterol by 25-hydroxycholesterol affects the interactions with sphingolipids: The Langmuir Monolayer Study complemented with theoretical calculations. <i>Journal of the Royal Society Interface</i> , 2021, 18, 20210050. | 1.5 | 6 |
| 14773 | Coulomb Explosion of Multi-charged Atomic Alkaline Metal Clusters. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2512-2517. | 1.1 | 1 |
| 14774 | Spectroscopic and DFT investigations of 8-hydroxy quinoline-5-sulfonic acid-5-chloro-8-hydroxyquinoline cocrystal. <i>Chemical Papers</i> , 2021, 75, 3387-3399. | 1.0 | 2 |
| 14775 | How Does Temperature Affect the Infrared Vibrational Spectra of Nanosized Silicate Dust?. <i>ACS Earth and Space Chemistry</i> , 2021, 5, 812-823. | 1.2 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 14776 | Designing Organic Electron Transport Materials for Stable and Efficient Performance of Perovskite Solar Cells: A Theoretical Study. <i>ACS Omega</i> , 2021, 6, 7086-7093. | 1.6 | 12 |
| 14777 | Exploring the Spatial Features of Electronic Transitions in Molecular and Biomolecular Systems by Swift Electrons. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2364-2373. | 2.3 | 1 |
| 14778 | A prochiral precursor in space? Accurate laboratory characterization of acetylacetylene in the cm-wave region. <i>Journal of Molecular Spectroscopy</i> , 2021, 377, 111441. | 0.4 | 4 |
| 14779 | A map of mass spectrometry-based <i>in silico</i> fragmentation prediction and compound identification in metabolomics. <i>Briefings in Bioinformatics</i> , 2021, 22, . | 3.2 | 18 |
| 14780 | Substituent Effects in Mechanochemical Allowed and Forbidden Cyclobutene Ring-Opening Reactions. <i>Journal of the American Chemical Society</i> , 2021, 143, 3846-3855. | 6.6 | 26 |
| 14781 | Modeling of the spectroscopy of core electrons with density functional theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1527. | 6.2 | 60 |
| 14782 | Atomic Evolution of Metal-Organic Frameworks into Co ₃ Coupling Vacancies by Cooperative Cascade Protection Strategy for Promoting Triiodide Reduction. <i>Journal of Physical Chemistry C</i> , 2021, 125, 6147-6156. | 1.5 | 13 |
| 14783 | Fluorescence quenching mechanism of 9-hydroxyphenal-1-one carbon quantum dots by Cu ²⁺ ions: An experimental and computational investigation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 408, 113103. | 2.0 | 4 |
| 14784 | Application of chemical derivatization techniques combined with chemical ionization mass spectrometry to detect stabilized Criegee intermediates and peroxy radicals in the gas phase. <i>Atmospheric Measurement Techniques</i> , 2021, 14, 2501-2513. | 1.2 | 5 |
| 14785 | The structure of dichlorotris(triphenylphosphine)ruthenium(II): a DFT study of interaction energies and substitution mechanism. <i>Molecular Simulation</i> , 0, , 1-8. | 0.9 | 1 |
| 14786 | Screening Nanographene-Mediated Inter(Porphyrin) Communication to Optimize Inter(Porphyrin-Fullerene) Forces. <i>Advanced Energy Materials</i> , 2021, 11, 2100158. | 10.2 | 9 |
| 14787 | Molecular Docking and Molecular Dynamics Simulation Studies of Triterpenes from <i>Vernonia patula</i> with the Cannabinoid Type 1 Receptor. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3595. | 1.8 | 10 |
| 14788 | Computational Analysis of the Interactions between the S100B Extracellular Chaperone and Its Amyloid β Peptide Client. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3629. | 1.8 | 6 |
| 14789 | Molecular engineering and the physisorption between (C ₂₄ H ₁₂) surface and Cl, F, P, S, Se and Zn atoms using DFT, B3LYP algorithms. <i>Materials Today: Proceedings</i> , 2021, , . | 0.9 | 0 |
| 14790 | [3.2.1] and [4.1.1] isomers of Lehn's [2.2.2] Cryptand: Prediction of ion selectivity by quantum chemical calculations XV**. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2021, 647, 915-921. | 0.6 | 3 |
| 14791 | Synthesis of All Thiophene-Based [7]Helicenes and Trithienothiepinines with Isomeric Location of Sulfur Atoms Based on Intramolecular Selectivity of Deprotonation. <i>Journal of Organic Chemistry</i> , 2021, 86, 4413-4422. | 1.7 | 12 |
| 14792 | Reactivity of Cu(I) Nacnac Complexes Toward Polypnictogen Compounds. <i>Inorganic Chemistry</i> , 2021, 60, 5840-5850. | 1.9 | 7 |
| 14793 | A posteriori corrections to the iterative qubit coupled cluster method to minimize the use of quantum resources in large-scale calculations. <i>Quantum Science and Technology</i> , 2021, 6, 024012. | 2.6 | 24 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14794 | An(III)/Ln(III) solvent extraction: Theoretical and experimental investigation of the role of ligand conformational mobility. <i>Journal of Molecular Liquids</i> , 2021, 325, 115098. | 2.3 | 16 |
| 14795 | Ternary Polymer Solar Cells with High Open Circuit Voltage containing Fullerene and New Thieno[3',2',6,7][1]Benzothieno[3,2- ϵ]Thieno[3,2- ϵ g][1]Benzothiophene-based Non-fullerene Small Molecules Acceptor. <i>Energy Technology</i> , 2021, 9, 2001100. | | 6 |
| 14796 | Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. <i>Applied Materials Today</i> , 2021, 22, 100924. | 2.3 | 57 |
| 14797 | Photochemical intermolecular dearomative cycloaddition of bicyclic azaarenes with alkenes. <i>Science</i> , 2021, 371, 1338-1345. | 6.0 | 119 |
| 14798 | Electrochemical Reduction Mechanism of $[(\eta^5-C_5H_5)_2Fe(dppf)(CO)]^+$ (dppf = 1,1'-bis(diphenylphosphino)ethane). <i>Journal of Physical Chemistry C</i> , 2021, 125, 577-587. | 1.1 | 5 |
| 14799 | Weakened Triplet-Triplet Annihilation of Diiodo-BODIPY Moieties without Influence on Their Intrinsic Triplet Lifetimes in Diiodo-BODIPY-Functionalized Pillar[5]arenes. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2344-2355. | 1.1 | 8 |
| 14800 | Computational study of oxidation mechanism of mineral green pigments. <i>Journal of Molecular Modeling</i> , 2021, 27, 108. | 0.8 | 0 |
| 14801 | Nickel-Sulfonate Mode of Substrate Binding for Forward and Reverse Reactions of Methyl-SCoM Reductase Suggest a Radical Mechanism Involving Long-Range Electron Transfer. <i>Journal of the American Chemical Society</i> , 2021, 143, 5481-5496. | 6.6 | 12 |
| 14802 | Quantum Mechanical Methods Predict Accurate Thermodynamics of Biochemical Reactions. <i>ACS Omega</i> , 2021, 6, 9948-9959. | 1.6 | 12 |
| 14803 | Theoretical studies on the electronic and optoelectronic properties of DNA/RNA hybrid-metal complexes. <i>Polyhedron</i> , 2021, 196, 115015. | 1.0 | 2 |
| 14804 | Structure, Bonding, and Photoaffinity Labeling Applications of Dialkyldiazirines. <i>Synlett</i> , 2021, 32, 1053-1059. | 1.0 | 7 |
| 14805 | Explaining and Fixing DFT Failures for Torsional Barriers. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2796-2804. | 2.1 | 23 |
| 14806 | A phenylalanine dynamic switch controls the interfacial activation of <i>Rhizopus chinensis</i> lipase. <i>International Journal of Biological Macromolecules</i> , 2021, 173, 1-12. | 3.6 | 27 |
| 14807 | Cobalt-Catalyzed Coupling of Aryl Chlorides with Aryl Boron Esters Activated by Alkoxides. <i>ACS Catalysis</i> , 2021, 11, 3856-3866. | 5.5 | 16 |
| 14808 | Assessing the Structure of Protic Ionic Liquids Based on Triethylammonium and Organic Acid Anions. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2781-2792. | 1.2 | 21 |
| 14810 | Theoretical Assessment of Hinge-Type Models for Electron Donors in Reaction Centers of Photosystems I and II as well as of Purple Bacteria. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3066-3079. | 1.2 | 6 |
| 14811 | A new series of Schiff base Ni(II) ₄ cubanes: Evaluation of magnetic coupling via carboxylate bridges. <i>Polyhedron</i> , 2021, 196, 115017. | 1.0 | 6 |
| 14812 | Designing and Screening High-Performance Non-Fullerene Acceptors: A Theoretical Exploration of Modified Y6. <i>Solar Rrl</i> , 2021, 5, 2100023. | 3.1 | 29 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14814 | Mechanistic Insights into the Nickel-Catalyzed Regioselective Carboxylation of Allylic Alcohols. <i>Organometallics</i> , 2021, 40, 869-879. | 1.1 | 15 |
| 14815 | Synthesis, spectral characterization, density functional theory studies, and biological screening of some transition metal complexes of a novel hydrazide-hydrazone ligand of isonicotinic acid. <i>Applied Organometallic Chemistry</i> , 2021, 35, e6205. | 1.7 | 20 |
| 14816 | AI-Active Chiral [3]Rotaxanes with Switchable Circularly Polarized Luminescence. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 9507-9515. | 7.2 | 95 |
| 14817 | Green Solvent-Based Perovskite Precursor Development for Ink-Jet Printed Flexible Solar Cells. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 3920-3930. | 3.2 | 23 |
| 14818 | Structural and Hydrolytic Stability of Coordinatively Unsaturated Metal-Organic Frameworks $M_3(BTC)_2$ (M = Cu, Co, Mn, Ni, and Zn): A Combined DFT and Experimental Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 5832-5847. | 1.5 | 11 |
| 14819 | Systematic Analysis of the Role of Substituents in Oxiranes, Oxetanes, and Oxathietanes Chemical Shifts. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2077-2087. | 1.1 | 1 |
| 14820 | Anti-quorum sensing activity in <i>Pseudomonas aeruginosa</i> PA01 of benzimidazolium salts: electronic, spectral and structural investigations as theoretical approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 6845-6856. | 2.0 | 12 |
| 14821 | From Chain- to Graphene-like Hydroxyl-terminated (ZnO) Clusters with $n=6$ Obtained via Zinc Dimethoxide Hydrolysis and Condensation: <i>Ab initio</i> Structural, Electronic, Vibrational and Optical Properties Calculations. <i>ChemPhysChem</i> , 2021, 22, 849-863. | 1.0 | 3 |
| 14822 | Inter/intramolecular hydrogen bonding mediate miscible blend formation between near-perfect alternating Poly(styrene- <i>alt</i> -hydroxyphenylmaleimide) copolymers and Poly(vinyl pyrrolidone). <i>Polymer</i> , 2021, 219, 123542. | 1.8 | 15 |
| 14823 | Electronic Structure Modification of Rectangular Phosphorene Quantum Dots Via Edge Passivation. <i>Journal of Physical Chemistry C</i> , 2021, 125, 5029-5036. | 1.5 | 4 |
| 14824 | Computational Investigation of Dichloromethane Ligand Substitution in the Enantiopure Cation $[(\text{C}_5\text{H}_5)_2\text{C}_5\text{H}_5\text{Re}(\text{NO})(\text{PPh}_3)_3(\text{ClCH}_2\text{Cl})]^+$ a Functional Equivalent of a Chiral Lewis Acid. <i>Organometallics</i> , 2021, 40, 742-759. | | 4 |
| 14825 | AI-Active Chiral [3]Rotaxanes with Switchable Circularly Polarized Luminescence. <i>Angewandte Chemie</i> , 2021, 133, 9593-9601. | 1.6 | 25 |
| 14826 | DFT Study on the Electrocatalytic Reduction of CO_2 to CO by a Molecular Chromium Complex. <i>Inorganic Chemistry</i> , 2021, 60, 3635-3650. | 1.9 | 18 |
| 14827 | Crystal Structure Determination of 4-[(Di- <i>p</i> -tolyl-amino)-benzylidene]-(5-pyridin-4-yl-[1,3,4]thiadiazol-2-yl)-imine along with Selected Properties of Imine in Neutral and Protonated Form with Camforosulphonic Acid: Theoretical and Experimental Studies. <i>Materials</i> , 2021, 14, 1952. | 1.3 | 2 |
| 14828 | Prebiotic Route to Thymine from Formamide—A Combined Experimental-Theoretical Study. <i>Molecules</i> , 2021, 26, 2248. | 1.7 | 1 |
| 14829 | Excited-state dynamics of $[\text{Mn}(\text{im})(\text{CO})_3(\text{phen})]^+$: PhotoCORM, catalyst, luminescent probe?. <i>Journal of Chemical Physics</i> , 2021, 154, 154102. | 1.2 | 8 |
| 14830 | Effects of Ionic Liquids on the Thermodynamics of Hydrogen Activation by Frustrated Lewis Pairs: A Density Functional Theory Study**. <i>ChemPhysChem</i> , 2021, 22, 968-974. | 1.0 | 2 |
| 14831 | Microwave spectrum and iodine nuclear quadrupole coupling constants of 1,1-diiodoethane. <i>Journal of Molecular Spectroscopy</i> , 2021, 378, 111419. | 0.4 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14832 | Cooperation/Competition between Halogen Bonds and Hydrogen Bonds in Complexes of 2,6-Diaminopyridines and X-CY3 (X = Cl, Br; Y = H, F). <i>Symmetry</i> , 2021, 13, 766. | 1.1 | 6 |
| 14833 | Thermochemistry of Gaseous Ytterbium and Gadolinium Hydroxides and Oxyhydroxides. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2913-2922. | 1.1 | 2 |
| 14834 | Ionization Energies and Dyson Orbitals of the Iso-electronic SO ₂ , O ₃ , and S ₃ Molecules from Electron Propagator Calculations. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3664-3680. | 1.1 | 3 |
| 14835 | Assessing the Accuracy of Local Hybrid Density Functional Approximations for Molecular Response Properties. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2928-2947. | 2.3 | 39 |
| 14836 | Phosphates branching effect on the structure, linear and NLO properties of linear phosphazenes. <i>Materials Chemistry and Physics</i> , 2021, 262, 124280. | 2.0 | 14 |
| 14837 | Fluorescence quenched and boosted by a-PET effect and host-guest complexation respectively in BODIPY-functionalized pillar[5]arene. <i>Dyes and Pigments</i> , 2021, 188, 109163. | 2.0 | 12 |
| 14838 | Enantioselective Construction of the Cycl[3.2.2]azine Core via Organocatalytic [12 + 2] Cycloadditions. <i>Journal of the American Chemical Society</i> , 2021, 143, 6140-6151. | 6.6 | 24 |
| 14839 | Assessment of SAPT and Supermolecular EDA Approaches for the Development of Separable and Polarizable Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2759-2774. | 2.3 | 20 |
| 14841 | Indium-Catalyzed Cycloisomerization of 1,6-Cyclohexenylalkynes. <i>Catalysts</i> , 2021, 11, 546. | 1.6 | 4 |
| 14842 | Direct Tracking Excited-State Intramolecular Charge Redistribution of Acceptor-Donor-Acceptor Molecule by Means of Femtosecond Stimulated Raman Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4456-4464. | 1.2 | 15 |
| 14843 | Structure Elucidation and Confirmation of Phloroglucinols from the Roots of <i>Garcinia dauphinensis</i> by Comparison of Experimental and Calculated ECD Spectra and Specific Rotations. <i>Journal of Natural Products</i> , 2021, 84, 1163-1174. | 1.5 | 2 |
| 14844 | Direct amination of naphthopurpurin and mompain, sea urchin pigments, and their O-methyl ethers by the reaction with ammonia. <i>Russian Chemical Bulletin</i> , 2021, 70, 792-804. | 0.4 | 2 |
| 14845 | Synthesis, structure, and properties of EuScCu ₃ and SrScCu ₃ . <i>Journal of Solid State Chemistry</i> , 2021, 296, 121926. | 1.4 | 15 |
| 14846 | First Direct Evidence of Interpartner Hydride/Deuteride Exchanges for Stored Sodiated Arginine/Fructose-6-phosphate Complex Anions within Salt-Solvated Structures. <i>Journal of the American Society for Mass Spectrometry</i> , 2021, 32, 1424-1440. | 1.2 | 4 |
| 14847 | Efficient Embedded Cluster Density Approximation Calculations with an Orbital-Free Treatment of Environments. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2737-2751. | 2.3 | 3 |
| 14848 | Electronic Structure and Vibrational Signatures of the Delocalized Radical in Hydrated Clusters of Copper(II) Hydroxide CuOH(H ₂ O) ₀₋₂ . <i>Journal of Physical Chemistry A</i> , 2021, 125, 3631-3645. | 1.1 | 3 |
| 14849 | Computational Study of Intramolecular Coordination Enhanced Oxidative Addition to form PdIV-Pincer Complexes, and Selectivity in Aryloxide Attack at PdIVCH ₂ CRR ² Motifs in Palladium-Mediated Organic Synthesis. <i>Organometallics</i> , 2021, 40, 1262-1269. | 1.1 | 3 |
| 14850 | Snapshots of the Fragmentation for C70@Single-Walled Carbon Nanotube: Tight-Binding Molecular Dynamics Simulations. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3929. | 1.8 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14851 | Mechanistic insights into the autocatalyzed rearrangement of 2-bromooxazolines to 2-bromoisocyanates by means of high-level quantum chemical methods. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4214. | 0.9 | 0 |
| 14852 | Tetraorganylargentate(III) Complexes: Key Intermediates in Silver-Mediated Cross-Coupling Reactions. <i>Organometallics</i> , 2021, 40, 2354-2363. | 1.1 | 11 |
| 14853 | Characterization of Triphenylamine and Ferrocenyl Donor- π -Donor Vinyl BODIPY Derivatives as Photoacoustic Contrast Agents. <i>Photochemistry and Photobiology</i> , 2021, , . | 1.3 | 2 |
| 14854 | Role of pH on Nanostructured SERS Active Substrates for Detection of Organic Dyes. <i>Molecules</i> , 2021, 26, 2360. | 1.7 | 3 |
| 14855 | The Oxidative Process of Acarbose, Maysin, and Luteolin with Maltase-Glucoamylase: Molecular Docking and Molecular Dynamics Study. <i>Applied Sciences (Switzerland)</i> , 2021, 11, 4067. | 1.3 | 1 |
| 14856 | Controlling and Fine-Tuning Charge-Transfer Emission in 2,6-Dicyanoaniline Multichromophores Prepared through Domino Reactions: Entry to a Potentially New Class of OLEDs. <i>Journal of Organic Chemistry</i> , 2021, 86, 6111-6125. | 1.7 | 7 |
| 14857 | Lewis Structures from Open Quantum Systems Natural Orbitals: Real Space Adaptive Natural Density Partitioning. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4013-4025. | 1.1 | 6 |
| 14858 | Crystal structure determination and computational studies of 1,4-dihydropyridine derivatives as selective T-type calcium channel blockers. <i>Journal of Molecular Structure</i> , 2021, 1230, 129898. | 1.8 | 8 |
| 14859 | Modeling Complex Solvent Effects on the Optical Rotation of Chiral Molecules: A Combined Molecular Dynamics and Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3095-3108. | 1.1 | 13 |
| 14860 | CHAL336 Benchmark Set: How Well Do Quantum-Chemical Methods Describe Chalcogen-Bonding Interactions?. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2783-2806. | 2.3 | 42 |
| 14861 | Small-Molecule Inhibitors of the RNA M6A Demethylases FTO Potently Support the Survival of Dopamine Neurons. <i>International Journal of Molecular Sciences</i> , 2021, 22, 4537. | 1.8 | 20 |
| 14862 | A full configuration interaction quantum Monte Carlo study of ScO, TiO, and VO molecules. <i>Journal of Chemical Physics</i> , 2021, 154, 164302. | 1.2 | 11 |
| 14863 | Sonication-assisted synthesis of a strawberry-like nano-structure triphenyltin(IV) adduct as precursor for preparation of nano-sized SnP2O7: Crystal structure and DFT calculations. <i>Journal of Molecular Structure</i> , 2021, 1230, 129630. | 1.8 | 0 |
| 14864 | Diradical character of the bond breaking in the reaction of Br ₂ with benzene: Reliable barriers using the CR-CC(2,3) method. <i>Computational and Theoretical Chemistry</i> , 2021, 1198, 113171. | 1.1 | 1 |
| 14865 | On the Mechanism of Dimerization of Stable Organic Radicals. <i>Russian Journal of Organic Chemistry</i> , 2021, 57, 506-514. | 0.3 | 1 |
| 14866 | Collision-induced dissociation of [UO ₂ (NO ₃)(O ₂)] ⁺ and reactions of product ions with H ₂ O and O ₂ . <i>Journal of Mass Spectrometry</i> , 2021, 56, e4720. | 0.7 | 1 |
| 14867 | Phototransformations of 2-aminonicotinic acid resolved with matrix isolation infrared spectroscopy and ab initio calculations. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 410, 113187. | 2.0 | 4 |
| 14868 | Quantum chemical calculation studies toward microscopic understanding of retention mechanism of Cs radioisotopes and other alkali metals in lichens. <i>Scientific Reports</i> , 2021, 11, 8228. | 1.6 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14869 | New D2R partial agonist candidates: an in silico approach from statistical models, molecular docking, and ADME/Tox properties. <i>Structural Chemistry</i> , 2021, 32, 2019-2033. | 1.0 | 1 |
| 14870 | Gas-Phase Experimental and Computational Studies of 5-Halouracils: Intrinsic Properties and Biological Implications. <i>Journal of Organic Chemistry</i> , 2021, 86, 6361-6370. | 1.7 | 5 |
| 14871 | Computational Study of Hydrogen Bond Interactions in Water Clusterâ€“Organic Molecule Complexes. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3369-3377. | 1.1 | 10 |
| 14872 | Expanding amphiphilic architectures by ring-opening of epoxides and polyepoxides with N-methyl-d-glucamine: Structure, chiral bias and gelation. <i>Carbohydrate Research</i> , 2021, 502, 108278. | 1.1 | 0 |
| 14873 | Computer-assisted evaluation of plant-derived Î²-secretase inhibitors in Alzheimerâ€™s disease. <i>Egyptian Journal of Medical Human Genetics</i> , 2021, 22, . | 0.5 | 8 |
| 14874 | Natural Gas Dehydration with Ionic-Liquid-Based Mixed Solvents. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 6033-6047. | 3.2 | 32 |
| 14875 | Solid Phase Nitrosylation of Enantiomeric Cobalt(II) Complexes. <i>Chemistry</i> , 2021, 3, 585-597. | 0.9 | 6 |
| 14876 | Experimental and density functional theory study of complexing agents on cobalt dissolution in alkaline solutions. <i>Electrochimica Acta</i> , 2021, 375, 137977. | 2.6 | 21 |
| 14877 | The thermochemical, structural, and spectroscopic analyses of the tautomers of sulfur and selenium modified emissive nucleobases. <i>Canadian Journal of Chemistry</i> , 2021, 99, 390-396. | 0.6 | 0 |
| 14878 | Solid-State Ionic Liquid: Key to Efficient Detection and Discrimination in Organic Semiconductor Gas Sensors. <i>ACS Applied Electronic Materials</i> , 2021, 3, 2152-2163. | 2.0 | 4 |
| 14879 | Light-Triggered Metal Coordination Dynamics in Photoswitchable Dithienyletheneâ€“Ferrocene System. <i>Inorganic Chemistry</i> , 2021, 60, 6086-6098. | 1.9 | 2 |
| 14880 | Enantioselectivity in the Noyoriâ€“Ikariya Asymmetric Transfer Hydrogenation of Ketones. <i>Organometallics</i> , 2021, 40, 1402-1410. | 1.1 | 24 |
| 14881 | Effects of edge substitution of subazaphenalenephthalocyanine with electron withdrawing and/or donating groups on electronic and optical properties: A DFT/TDDFT study. <i>Materials Chemistry and Physics</i> , 2021, 263, 124420. | 2.0 | 4 |
| 14882 | A Trögerâ€™s Base-Derived Covalent Organic Polymer Containing Carbazole Units as a High-Performance Supercapacitor. <i>Polymers</i> , 2021, 13, 1385. | 2.0 | 32 |
| 14884 | Active discovery of organic semiconductors. <i>Nature Communications</i> , 2021, 12, 2422. | 5.8 | 66 |
| 14885 | Methane Overâ€“Oxidation by Extraâ€“Framework Copperâ€“Oxo Active Sites of Copperâ€“Exchanged Zeolites: Crucial Role of Traps for the Separated Methyl Group. <i>ChemPhysChem</i> , 2021, 22, 1101-1109. | 1.0 | 7 |
| 14886 | Multi-replica biased sampling for photoswitchable Î¶-conjugated polymers. <i>Journal of Chemical Physics</i> , 2021, 154, 174108. | 1.2 | 6 |
| 14887 | Carbon and Nitrogen K-Edge NEXAFS Spectra of Indole, 2,3-Dihydro-7-azaindole, and 3-Formylindole. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4160-4172. | 1.1 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14888 | Phase Transformations of Azithromycin Crystals Investigated by Thermal and Spectroscopic Analyses Combined with <i>Ab Initio</i> Calculations. <i>Crystal Growth and Design</i> , 2021, 21, 3602-3613. | 1.4 | 3 |
| 14889 | The Effect of Remote Donor Substituents on the Properties of Alkoxy and Amino Fischer Carbene Complexes of Tungsten. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2021, 647, 1152-1164. | 0.6 | 2 |
| 14890 | Tuning the Gold(I)-Carbon σ Bond in Gold-Alkynyl Complexes through Structural Modifications of the NHC Ancillary Ligand: Effect on Spectroscopic Observables and Reactivity. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 2401-2416. | 1.0 | 5 |
| 14891 | Zinc- and Cadmium meso-aryl porphyrins: Non-aromatic NIR Dyes with Distinct Conformational Features. <i>Chemistry - A European Journal</i> , 2021, 27, 8021-8029. | 1.7 | 2 |
| 14892 | Molecular Simulation of High-Salinity Brines in Contact with Diisopropylamine and Tripropylamine Solvents. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 7917-7925. | 1.8 | 10 |
| 14893 | Silver (I)-dimercaptotriazine functionalized silica: A highly selective liquid chromatography stationary phase targeting unsaturated molecules. <i>Journal of Chromatography A</i> , 2021, 1645, 462122. | 1.8 | 6 |
| 14894 | Infrared spectra of neutral polycyclic aromatic hydrocarbons based on machine learning potential energy surface and dipole mapping. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1. | 0.5 | 6 |
| 14895 | Water-oriented magnetic anisotropy transition. <i>Nature Communications</i> , 2021, 12, 2738. | 5.8 | 12 |
| 14896 | ParAMS: Parameter Optimization for Atomistic and Molecular Simulations. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3737-3743. | 2.5 | 9 |
| 14897 | Electronic structure and reactivity of tirapazamine as a radiosensitizer. <i>Journal of Molecular Modeling</i> , 2021, 27, 177. | 0.8 | 2 |
| 14898 | Fluorescent Indolo[3,2- <i>a</i>]phenazines against <i>Toxoplasma gondii</i> : Concise Synthesis by Gold-Catalyzed Cycloisomerization with 1,2-Silyl Migration and <i>ipso</i> -iodination Suzuki Sequence. <i>Chemistry - A European Journal</i> , 2021, 27, 9774-9781. | 1.7 | 2 |
| 14899 | Kinetics of Azanone (HNO) Reactions with Thiols: Effect of pH. <i>Cell Biochemistry and Biophysics</i> , 2021, 79, 845-856. | 0.9 | 4 |
| 14900 | A new metal-organic framework of 3,9-diazatetraasterane-1,5,7,11-tetracarboxylic acid-3,6,9,12-tetraphenyl with sodium ion: Synthesis, characterization and DFT calculations. <i>Chemical Physics Letters</i> , 2021, 771, 138469. | 1.2 | 4 |
| 14901 | Discovering chemical reaction pathways using accelerated molecular dynamics simulations and network analysis tools - Application to oxidation induced decomposition of ethylene carbonate. <i>Chemical Physics Letters</i> , 2021, 770, 138439. | 1.2 | 7 |
| 14902 | Trends in Conjugated Chalcogenophenes: A Theoretical Study. <i>Chemistry - A European Journal</i> , 2021, 27, 9038-9043. | 1.7 | 13 |
| 14903 | Arylethynyl Helices Supported by π -Stacking and Halogen Bonding. <i>ChemPlusChem</i> , 2021, 86, 745-749. | 1.3 | 1 |
| 14904 | Structures of a non-ribosomal peptide synthetase condensation domain suggest the basis of substrate selectivity. <i>Nature Communications</i> , 2021, 12, 2511. | 5.8 | 53 |
| 14905 | Harmonic Infrared and Raman Spectra in Molecular Environments Using the Polarizable Embedding Model. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3599-3617. | 2.3 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14906 | Quantum chemical investigation on D-Ï-A-based phenothiazine organic chromophores with spacer and electron acceptor effects for DSSCs. <i>Structural Chemistry</i> , 2021, 32, 2199-2207. | 1.0 | 4 |
| 14907 | Bifunctional Primary Amino-Ï-thiourea Asymmetric Catalysis: The Imine-Ïminium Ion Mechanism in the Michael Addition of Nitromethane to Enone. <i>Asian Journal of Organic Chemistry</i> , 2021, 10, 1472-1485. | 1.3 | 12 |
| 14908 | A guide to benchmarking enzymatically catalysed reactions: the importance of accurate reference energies and the chemical environment. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1. | 0.5 | 6 |
| 14909 | Contribution of the Molecular Fluorophore IPCA to Excitation-Independent Photoluminescence of Carbon Dots. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12140-12148. | 1.5 | 22 |
| 14910 | Significance Of Nuclear Quantum Effects In Hydrogen Bonded Molecular Chains. <i>ACS Nano</i> , 2021, 15, 10357-10365. | 7.3 | 11 |
| 14911 | Reference Energies for Intramolecular Charge-Transfer Excitations. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3666-3686. | 2.3 | 51 |
| 14912 | Theoretical design of Salen-Ï-metal-based materials for highly selective separation of C ₂ H ₂ /C ₂ H ₄ . <i>Chemical Physics Letters</i> , 2021, 771, 138523. | 1.2 | 0 |
| 14913 | Theoretical and Experimental Vibrational Characterization of Biologically Active Nd(III) Complex. <i>Molecules</i> , 2021, 26, 2726. | 1.7 | 1 |
| 14914 | Computational insights into electrochemical cross-Ï-coupling of quaternary borate salts. <i>Electrochemical Science Advances</i> , 0, , e2100032. | 1.2 | 1 |
| 14915 | Isolation of Neutral, Mono-Ï, and Dicationic B ₂ P ₂ Rings by Diphosphorus Addition to a Boron-Ï-Boron Triple Bond. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 13661-13665. | 7.2 | 9 |
| 14916 | Isolierung neutraler, mono-Ï- und dikationischer B ₂ P ₂ -Ï-Ringe durch Addition eines Diphosphans an eine Bor-Ï-Dreifachbindung. <i>Angewandte Chemie</i> , 2021, 133, 13774-13779. | 1.6 | 2 |
| 14917 | Recent advancement on the mechanism of olefin metathesis by Grubbs catalysts: A computational perspective. <i>Polyhedron</i> , 2021, 200, 115096. | 1.0 | 9 |
| 14918 | Erosion of refractory carbides in high-Ï-temperature hydrogen from ab initio computations. <i>Journal of the American Ceramic Society</i> , 2021, 104, 4695-4707. | 1.9 | 2 |
| 14919 | Density Functional Theory Calculations of Core-Ï-Electron Binding Energies at the K-Edge of Heavier Elements. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3644-3651. | 2.3 | 8 |
| 14920 | Formation and thermal stability of supramolecular complexes of dibromosubstituted zinc(II) dipyrromethenate with ethanol and N,N-Ï-dimethylformamide. <i>Thermochimica Acta</i> , 2021, 699, 178911. | 1.2 | 3 |
| 14921 | Superhalogens Among 3^d-Metal Compounds: ^MF₄, ^MF₆, ^MF₁₂, and ^MF₁₈ (^M = Sc-Ï-Zn). <i>Journal of Physical Chemistry A</i> , 2021, 125, 4409-4419. | 1.1 | 2 |
| 14922 | DFT Approach for Predicting ¹³C NMR Shifts of Atoms Directly Coordinated to Nickel. <i>Organometallics</i> , 2021, 40, 1614-1625. | 1.1 | 8 |
| 14923 | Computational Studies on Reactions of Some Organic Azides with C-Ï-H Bonds. <i>ChemistrySelect</i> , 2021, 6, 4368-4381. | 0.7 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14924 | Role of nitrogen doping in stoichiometric and defective carbon nano-onions: Structural diversity from DFT calculations. <i>Carbon</i> , 2021, 176, 198-208. | 5.4 | 16 |
| 14925 | Achieving Purely Organic Room-Temperature Phosphorescence Mediated by a Host-Guest Charge Transfer State. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4600-4608. | 2.1 | 47 |
| 14926 | Converged Structural and Spectroscopic Properties for Refined QM/MM Models of Azurin. <i>Inorganic Chemistry</i> , 2021, 60, 7399-7412. | 1.9 | 10 |
| 14927 | Inhibition of cyclooxygenase by blocking the reducing cosubstrate at the peroxidase site: Discovery of galangin as a novel cyclooxygenase inhibitor. <i>European Journal of Pharmacology</i> , 2021, 899, 174036. | 1.7 | 7 |
| 14928 | Meso-nitro substitution as a means of Mn-octaethylporphyrin redox state controlling. <i>Journal of Organometallic Chemistry</i> , 2021, 940, 121790. | 0.8 | 1 |
| 14929 | Polarizability of atomic Pt, Pt ⁺ , and Pt ²⁺ . <i>Journal of Chemical Physics</i> , 2021, 154, 174302. | 1.2 | 2 |
| 14930 | Robust, Enantioselective Construction of Challenging, Biologically Relevant Tertiary Ether Stereocenters. <i>ACS Catalysis</i> , 2021, 11, 6325-6333. | 5.5 | 17 |
| 14931 | Estimation of the reducing power and electrochemical behavior of few flavonoids and polyhydroxybenzophenones substantiated by bond dissociation energy: a comparative analysis. <i>Molecular Diversity</i> , 2022, 26, 1101-1113. | 2.1 | 8 |
| 14932 | How Many Electrons Does a Molecular Electride Hold?. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4819-4835. | 1.1 | 7 |
| 14933 | Through Positional Isomerism: Impact of Molecular Composition on Enhanced Triplet Harvest for Solution-Processed OLED Efficiency Improvement. <i>ACS Applied Electronic Materials</i> , 2021, 3, 2317-2332. | 2.0 | 14 |
| 14934 | A Singular Molecule-to-Molecule Transformation on Video: The Bottom-Up Synthesis of Fullerene C ₆₀ from Truxene Derivative C ₆₀ H ₃₀ . <i>ACS Nano</i> , 2021, 15, 12804-12814. | 7.3 | 18 |
| 14935 | High-temperature binding parameters and molecular dynamics of 4-hydroxybenzoic acid and β -casein complexes, determined via the method of continuous variation and fluorescence spectroscopy. <i>Food Hydrocolloids</i> , 2021, 114, 106567. | 5.6 | 14 |
| 14936 | Pd on nitrogen rich polymer-halloysite nanocomposite as an environmentally benign and sustainable catalyst for hydrogenation of polyalphaolefin based lubricants. <i>Journal of Industrial and Engineering Chemistry</i> , 2021, 97, 441-451. | 2.9 | 47 |
| 14937 | Insight into the effect of He atmospheric pressure plasma jets on low-density polyethylene surfaces by fixed-point treatment. <i>Journal Physics D: Applied Physics</i> , 2021, 54, 285204. | 1.3 | 10 |
| 14938 | Wettability Reversal on Dolomite Surfaces by Divalent Ions and Surfactants: An Experimental and Molecular Dynamics Simulation Study. <i>Langmuir</i> , 2021, 37, 6641-6649. | 1.6 | 20 |
| 14939 | Synthesis, Structure, and Spectroscopic Study of Redox-Active Heterometallic Cluster-Based Complexes [Re ₅ MoSe ₈ (CN) ₆] ⁿ . <i>Inorganic Chemistry</i> , 2021, 60, 8838-8850. | 1.9 | 4 |
| 14940 | Investigation of charge transfer interaction in heterometallic precursors to control their surface reactivity for MOCVD of Pd-Cu alloy films. <i>Applied Surface Science</i> , 2021, 547, 149068. | 3.1 | 2 |
| 14941 | Optical and structural properties of cyanine dyes via electronic structure calculations. <i>Computational and Theoretical Chemistry</i> , 2021, 1199, 113197. | 1.1 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 14942 | Analysis of Noninnocence of Phosphaquinodimethane Ligands when Charge and Aromaticity Come into Play. <i>Chemistry - A European Journal</i> , 2021, 27, 9350-9359. | 1.7 | 4 |
| 14943 | Cation-Anion Interactions, Stability, and IR Spectra of Dicationic Amino Acid-Based Ionic Liquids Probed Using Density Functional Theory. <i>Journal of Molecular Modeling</i> , 2021, 27, 180. | 0.8 | 4 |
| 14944 | Synthesis and structural characterizations of Pd(II) complexes bearing the new hexahydropyrimidine and tetrahydropyrimidinium based bis(pyrazole) ligands with DFT studies. <i>Journal of Molecular Structure</i> , 2021, 1231, 129949. | 1.8 | 3 |
| 14945 | Understanding the Steric Structures of Dicarboxylate Ions Incorporated in Octacalcium Phosphate Crystals. <i>Materials</i> , 2021, 14, 2703. | 1.3 | 5 |
| 14946 | The aug-cc-pVTZ basis set for the p-block fourth-row elements Ga, Ge, As, Se, and Br. <i>Magnetic Resonance in Chemistry</i> , 2021, 59, 1134-1145. | 1.1 | 6 |
| 14947 | Halogen bond interaction: Role of hybridization and induction. <i>Chemical Physics Letters</i> , 2021, 771, 138522. | 1.2 | 6 |
| 14948 | Theoretical investigations on the antioxidant potential of a non-phenolic compound thymoquinone: a DFT approach. <i>Journal of Molecular Modeling</i> , 2021, 27, 173. | 0.8 | 13 |
| 14949 | On the Use of Normalized Metrics for Density Sensitivity Analysis in DFT. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4639-4652. | 1.1 | 7 |
| 14950 | Multiscale Quantum Refinement Approaches for Metalloproteins. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3783-3796. | 2.3 | 8 |
| 14951 | Quantum Chemistry Calculations for Metabolomics. <i>Chemical Reviews</i> , 2021, 121, 5633-5670. | 23.0 | 47 |
| 14952 | Non-classical disproportionation revealed by photo-chemically induced dynamic nuclear polarization NMR. <i>Magnetic Resonance</i> , 2021, 2, 281-290. | 0.8 | 10 |
| 14953 | Theoretical Study of Electronic Structure of Charged Fullerenes. <i>Journal of Nanomaterials</i> , 2021, 2021, 1-10. | 1.5 | 1 |
| 14954 | A DFT simulation on induction reactions involved radicals during pyrolysis of heavy organics. <i>Journal of Fuel Chemistry and Technology</i> , 2021, 49, 684-693. | 0.9 | 4 |
| 14955 | Computational studies on binding, solvent, and pH effects on (S)-propranolol and methacrylic acid complex. <i>Journal of Molecular Modeling</i> , 2021, 27, 153. | 0.8 | 0 |
| 14956 | Topology Effects in Molecular Organic Electronic Materials: Pyrene and Azupyrene**. <i>ChemPhysChem</i> , 2021, 22, 1065-1073. | 1.0 | 15 |
| 14957 | Chelating Guanidines for Dysprosium(III) Single-Molecule Magnets. <i>Chinese Journal of Chemistry</i> , 2021, 39, 1635-1640. | 2.6 | 7 |
| 14958 | Investigation of tautomerism of 1,3,5-triazine derivative, stability, and acidity of its tautomers from density functional theory. <i>Journal of Molecular Modeling</i> , 2021, 27, 147. | 0.8 | 3 |
| 14960 | Intramolecular hydrogen-bonding effects on structural and electronic properties of pyrrole-furan derivatives: a density functional calculation. <i>Optical and Quantum Electronics</i> , 2021, 53, 1. | 1.5 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 14961 | Revisiting stacking interactions in tetrathiafulvalene and selected derivatives using tight-binding quantum chemical calculations and local coupled-cluster method. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 311-320. | 0.5 | 6 |
| 14962 | A Stable Homoleptic Divinyl Tetrelene Series. <i>Chemistry - A European Journal</i> , 2021, 27, 8572-8579. | 1.7 | 25 |
| 14963 | Enhancing Thermopower and Nernst Signal of High-Mobility Dirac Carriers by Fermi Level Tuning in the Layered Magnet EuMnBi_2 . <i>Advanced Functional Materials</i> , 2021, 31, 2102275. | 7.8 | 8 |
| 14964 | Functionalized Au ₁₅ nanoclusters as luminescent probes for protein carbonylation detection. <i>Communications Chemistry</i> , 2021, 4, . | 2.0 | 16 |
| 14965 | Rational Design of Novel Anticancer Small-Molecule RNA m6A Demethylase ALKBH5 Inhibitors. <i>ACS Omega</i> , 2021, 6, 13310-13320. | 1.6 | 57 |
| 14966 | Organocatalytic Asymmetric Multicomponent Cascade Reaction for the Synthesis of Contiguously Substituted Tetrahydronaphthols. <i>Journal of the American Chemical Society</i> , 2021, 143, 8208-8220. | 6.6 | 16 |
| 14967 | Interaction Region Indicator: A Simple Real Space Function Clearly Revealing Both Chemical Bonds and Weak Interactions**. <i>Chemistry Methods</i> , 2021, 1, 231-239. | 1.8 | 516 |
| 14968 | Cu(I) complexes designed on 2-pyrimidylphosphine and 1,4-dicyanobenzene: Synthesis and thermally activated delayed fluorescence. <i>Inorganica Chimica Acta</i> , 2021, 521, 120347. | 1.2 | 9 |
| 14969 | Multistructural Variational Reaction Kinetics of the Simplest Unsaturated Methyl Ester: H-Abstraction from Methyl Acrylate by H, OH, CH ₃ , and HO ₂ Radicals. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5103-5116. | 1.1 | 11 |
| 14970 | Significant Enhancement of the Polarization Holographic Performance of Photopolymeric Materials by Introducing Graphene Oxide. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 27500-27512. | 4.0 | 25 |
| 14971 | A density functional theory study of Fe(II)/Fe(III) distribution in single layer green rust: a cluster approach. <i>Geochemical Transactions</i> , 2021, 22, 3. | 1.8 | 2 |
| 14972 | Antimicrobial, antimalarial, and cytotoxic substances from the insect pathogenic fungus <i>Beauveria asiatica</i> BCC 16812. <i>Phytochemistry Letters</i> , 2021, 43, 8-15. | 0.6 | 4 |
| 14973 | A soft x-ray probe of a titania photoelectrode sensitized with a triphenylamine dye. <i>Journal of Chemical Physics</i> , 2021, 154, 234707. | 1.2 | 2 |
| 14974 | Non-noble metal single atom catalysts with S, N co-doped defective graphene support: A theoretical study of highly efficient acetylene hydration. <i>Materials Today Communications</i> , 2021, 27, 102216. | 0.9 | 2 |
| 14975 | Intramolecular H-Bond Dynamics of Catechol Investigated by THz High-Resolution Spectroscopy of Its Low-Frequency Modes. <i>Molecules</i> , 2021, 26, 3645. | 1.7 | 9 |
| 14976 | NMR Indirect Spin-Spin Coupling Constants in a Modern Quasi-Relativistic Density Functional Framework. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3974-3994. | 2.3 | 27 |
| 14977 | Simple route to lithium dendrite prevention for long cycle-life lithium metal batteries. <i>Applied Materials Today</i> , 2021, 23, 101062. | 2.3 | 8 |
| 14978 | The Sulfolene Protecting Group: Observation of a Direct Photoinitiated Cheletropic Ring Opening. <i>ChemPhotoChem</i> , 2021, 5, 863-870. | 1.5 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14979 | Facile Fabrication of Functionalized Separators for Lithium-Ion Batteries with Ionic Conduction Path Modifications via the $\text{I}^{137}\text{-Ray}$ Co-irradiation Grafting Process. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 27663-27673. | 4.0 | 12 |
| 14980 | Zinc Stabilized Azo-anion Radical in Dehydrogenative Synthesis of N-Heterocycles. An Exclusively Ligand Centered Redox Controlled Approach. <i>ACS Catalysis</i> , 2021, 11, 7498-7512. | 5.5 | 42 |
| 14981 | Shermo: A general code for calculating molecular thermochemistry properties. <i>Computational and Theoretical Chemistry</i> , 2021, 1200, 113249. | 1.1 | 331 |
| 14982 | Using Density Functional Theory to Correlate Charge Transport Properties with Gas Sensing by Organic Nanowires. <i>ACS Applied Nano Materials</i> , 2021, 4, 5972-5980. | 2.4 | 5 |
| 14983 | $\text{P}^{\delta-}\text{O}^{\delta-}\text{N}$ Bridged Cu(I) Dimers Featuring Both TADF and Phosphorescence. From Overview towards Detailed Case Study of the Excited Singlet and Triplet States. <i>Molecules</i> , 2021, 26, 3415. | 1.7 | 9 |
| 14984 | Probing the Spin State of Spin-Crossover Complexes on Surfaces with Vacuum Ultraviolet Angle-Resolved Photoemission Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2021, 125, 14105-14116. | 1.5 | 3 |
| 14985 | QM/MM Study of Human Transketolase: Thiamine Diphosphate Activation Mechanism and Complete Catalytic Cycle. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3502-3515. | 2.5 | 4 |
| 14986 | Study on the dissolution of aluminium carbide formed on the graphite cathode in aluminium electrolysis. <i>Journal of Molecular Liquids</i> , 2021, 331, 115767. | 2.3 | 2 |
| 14987 | Catalytic asymmetric nucleophilic fluorination using $\text{BF}_3 \cdot \text{Et}_2\text{O}$ as fluorine source and activating reagent. <i>Nature Communications</i> , 2021, 12, 3957. | 5.8 | 27 |
| 14988 | The Effect of Added Ligands on the Reactions of $[\text{Ni}(\text{COD})(\text{dppf})]$ with Alkyl Halides: Halide Abstraction May Be Reversible. <i>Organometallics</i> , 2021, 40, 1997-2007. | 1.1 | 12 |
| 14989 | Quantitative structure-activity relationship and machine learning studies of 2-thiazolylhydrazone derivatives with anti- <i>Cryptococcus neoformans</i> activity. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 9789-9800. | 2.0 | 2 |
| 14990 | Computational Chemistry: The Exciting Opportunities and the Boring Details. <i>Israel Journal of Chemistry</i> , 2022, 62, . | 1.0 | 5 |
| 14991 | Reduced Two-Electron Interactions in Anharmonic Molecular Vibrational Calculations Involving Localized Normal Coordinates. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4383-4391. | 2.3 | 1 |
| 14992 | Mn(III) complexes with nitro-substituted ligands—Spin states with a twist. <i>Journal of Applied Physics</i> , 2021, 129, . | 1.1 | 12 |
| 14993 | Corrosion inhibition properties of small peptides: DFT and Monte Carlo simulation studies. <i>Journal of Molecular Liquids</i> , 2021, 331, 115782. | 2.3 | 27 |
| 14994 | Experimental and DFT study on titanium-based half-sandwich metallocene catalysts and their application for production of 1-hexene from ethylene. <i>Molecular Catalysis</i> , 2021, 509, 111636. | 1.0 | 12 |
| 14995 | Hexagonal Cylinder Mesoporous Sorbent for Separation of Uranium Ions from Nitrate Media. <i>Chemical Engineering and Technology</i> , 2021, 44, 1470-1478. | 0.9 | 6 |
| 14996 | Mechanosynthesis of Eutectics of Anti-inflammatory Drug Ethenzamide—A Comparison with Analogous Cocrystals. <i>Chemistry Methods</i> , 2021, 1, 408-414. | 1.8 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 14997 | The pH and mercury ion stimuli-responsive supramolecular assemblies of cucurbit[7]uril and Hoechst 33342. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 254, 119656. | 2.0 | 6 |
| 14998 | Adsorption of the drug bempedoic acid over different 2D/3D nanosurfaces and enhancement of Raman activity enabling ultrasensitive detection: First principle analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 254, 119630. | 2.0 | 12 |
| 14999 | Interaction studies of glycine, acetate and methylamine on β -tellurene nanoribbon – A first-principles analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 105, 107895. | 1.3 | 15 |
| 15000 | Growth, structural, Hirshfeld surface analysis, DFT validation on the crystal structure of 1, 10-Phenanthroline-1,10-dione perchlorate monohydrate. <i>Chemical Data Collections</i> , 2021, 33, 100706. | 1.1 | 1 |
| 15001 | General Perturb-Then-Diagonalize Model for the Vibrational Frequencies and Intensities of Molecules Belonging to Abelian and Non-Abelian Symmetry Groups. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4332-4358. | 2.3 | 15 |
| 15002 | Learning Molecular Representations for Thermochemistry Prediction of Cyclic Hydrocarbons and Oxygenates. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5166-5179. | 1.1 | 10 |
| 15003 | From Oligo(Phenyleneethynylene) Monomers to Supramolecular Helices: The Role of Intermolecular Interactions in Aggregation. <i>Molecules</i> , 2021, 26, 3530. | 1.7 | 2 |
| 15004 | Optical Response of Sila-Fullerenes in Interaction With Glycoproteins for Environmental Monitoring. <i>Frontiers in Physics</i> , 2021, 9, . | 1.0 | 2 |
| 15005 | Comparing molecular and electronic properties of perylene tetracarboxylic diimides decorated at 1,6- and 1,7-bay-positions using DFT/TDDFT method. <i>Materials Today Communications</i> , 2021, 27, 102446. | 0.9 | 1 |
| 15006 | Dissecting Transmetalation Reactions at the Molecular Level: Role of the Coordinated Anion in Gas-Phase Models for the Transmetalation Step of the Miyaura Cross-Coupling Reaction. <i>Organometallics</i> , 2021, 40, 1822-1829. | 1.1 | 5 |
| 15007 | Ground-State Structures of Hydrated Calcium Ion Clusters From Comprehensive Genetic Algorithm Search. <i>Frontiers in Chemistry</i> , 2021, 9, 637750. | 1.8 | 6 |
| 15008 | On-Site Detection of SARS-CoV-2 Antigen by Deep Learning-Based Surface-Enhanced Raman Spectroscopy and Its Biochemical Foundations. <i>Analytical Chemistry</i> , 2021, 93, 9174-9182. | 3.2 | 58 |
| 15009 | Copper-Oxo Active Sites for Methane C-H Activation in Zeolites: Molecular Understanding of Impact of Methane Hydroxylation on UV-Vis Spectra. <i>Inorganic Chemistry</i> , 2021, 60, 8489-8499. | 1.9 | 11 |
| 15010 | Unexpected Formation of the Highly Symmetric Borate Ion $[B(SiCl_3)_4]^{-}$. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 2583-2594. | 1.0 | 4 |
| 15011 | A tautomeric ligand enables directed C-H hydroxylation with molecular oxygen. <i>Science</i> , 2021, 372, 1452-1457. | 6.0 | 84 |
| 15012 | Evaluation of density functional theory for a large and diverse set of organic and inorganic equilibrium structures. <i>Journal of Computational Chemistry</i> , 2021, 42, 1590-1601. | 1.5 | 44 |
| 15013 | Effects of insecticide acephate on membrane mimetic systems: The role played by electrostatic interactions with lipid polar headgroups. <i>Journal of Molecular Liquids</i> , 2021, 332, 115868. | 2.3 | 12 |
| 15014 | Study of Ground State Interactions of Enantiopure Chiral Quaternary Ammonium Salts and Amides, Nitroalkanes, Nitroalkenes, Esters, Heterocycles, Ketones and Fluoroamides. <i>Chemistry - A European Journal</i> , 2021, 27, 11352-11366. | 1.7 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15015 | The Synthesis of a Bis(thiosemicarbazone) Macrocyclic Ligand and the Mn(II), Co(II), Zn(II) and ⁶⁸ Ga(III) Complexes. <i>Molecules</i> , 2021, 26, 3646. | 1.7 | 6 |
| 15016 | Through Bridge Spin Coupling in Homo- and Heterobimetallic Porphyrin Dimers upon Stepwise Oxidations: A Spectroscopic and Theoretical Investigation. <i>Chemistry - A European Journal</i> , 2021, 27, 11428-11441. | 1.7 | 4 |
| 15017 | Performance of the DLPNO-CCSD and recent DFT methods in the calculation of isotropic and dipolar contributions to ¹⁴ N hyperfine coupling constants of nitroxide radicals. <i>Journal of Molecular Modeling</i> , 2021, 27, 194. | 0.8 | 3 |
| 15018 | Quantum chemistry for molecules at extreme pressure on graphical processing units: Implementation of extreme-pressure polarizable continuum model. <i>Journal of Chemical Physics</i> , 2021, 154, 244103. | 1.2 | 4 |
| 15019 | Discussion on the dimerization reaction of penicillin antibiotics. <i>Journal of Pharmaceutical Analysis</i> , 2022, 12, 481-488. | 2.4 | 2 |
| 15020 | Combined experimental and computational study on the role of ionic liquid containing ligand in the catalytic performance of halloysite-based hydrogenation catalyst. <i>Journal of Molecular Liquids</i> , 2021, 331, 115740. | 2.3 | 35 |
| 15021 | The evaluation of anchoring processes and chemical stability of zwitterionic molecules via local reactivity indexes. <i>Computational Materials Science</i> , 2021, 193, 110418. | 1.4 | 2 |
| 15022 | Perturbation approach to constrained electron transfer in density functional theory. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1. | 0.5 | 1 |
| 15023 | Mechanism of Counterion-Controlled Regioselective Hydrothiolation of 1,3-Dienes: Insights from a Density Functional Theory Study. <i>ACS Catalysis</i> , 2021, 11, 7659-7671. | 5.5 | 2 |
| 15024 | Theoretical Study of Effects of Solvents, Ligands, and Anions on Separation of Trivalent Lanthanides and Actinides. <i>Inorganic Chemistry</i> , 2021, 60, 9552-9562. | 1.9 | 14 |
| 15025 | A Halomanganates(II) with P, P- TM -Diprotonated Bis(2-Diphenylphosphinophenyl)ether: Wavelength-Excitation Dependence of the Quantum Yield and Role of the Non-Covalent Interactions. <i>International Journal of Molecular Sciences</i> , 2021, 22, 6873. | 1.8 | 8 |
| 15026 | 1,3,4,5-Tetraamino-1,2,4-triazolium Cation: An Energetic Moiety. <i>Inorganic Chemistry</i> , 2021, 60, 9645-9652. | 1.9 | 9 |
| 15027 | Molecular Dynamics and Emerging Network Graphs of Interactions in Dinitrile-Based Li-Ion Battery Electrolytes. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7231-7240. | 1.2 | 3 |
| 15028 | Identification of reaction path for the synthesis of polyoxymethylene dimethyl ethers from methanol and paraformaldehyde catalyzed by Al-MCM-41 zeolite. <i>Computational and Theoretical Chemistry</i> , 2021, 1200, 113248. | 1.1 | 2 |
| 15029 | Micro-Aqueous Organic System: A Neglected Model in Computational Lipase Design?. <i>Biomolecules</i> , 2021, 11, 848. | 1.8 | 2 |
| 15030 | The synergy of CHEF and ICT toward fluorescence "turn-on" probes based on push-pull benzothiazoles for selective detection of Cu ²⁺ in acetonitrile/water mixture. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 415, 113318. | 2.0 | 15 |
| 15031 | Direct Conversion of Alginate Oligo- and Polysaccharides into Biodegradable and Non-Ecotoxic Anionic Furanic Surfactants: An Experimental and Mechanistic Study. <i>Advanced Sustainable Systems</i> , 2021, 5, 2100108. | 2.7 | 5 |
| 15032 | A comparative study on surface/interface mechanism and antibacterial properties of different hybrid materials prepared with essential oils active ingredients and palygorskite. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 618, 126455. | 2.3 | 16 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 15033 | Insights into complexation and enantioselectivity of uranyl- β -(2-hydroxy-3-methoxyphenyl)- α -(2-hydroxyphenyl)thiopyrano[3,2- <i>h</i>]thiochromene-4,7-dione with R/S organophosphorus pesticides. Applied Organometallic Chemistry, 2021, 35, e6331. | 4.1 | 31 |
| 15034 | Super selective ammonia separation through multiple-site interaction with ionic liquid-based hybrid membranes. Journal of Membrane Science, 2021, 628, 119264. | 2.3 | 18 |
| 15035 | Wettability alteration by Smart Water multi-ion exchange in carbonates: A molecular dynamics simulation study. Journal of Molecular Liquids, 2021, 332, 115830. | 5.4 | 10 |
| 15036 | Permeation of chemisorbed hydrogen through graphene: A flipping mechanism elucidated. Carbon, 2021, 178, 718-727. | 5.3 | 6 |
| 15037 | Effects of structural distortion on the optoelectronic properties and reactivity of fullerenes: a DFT study. Journal of Nanostructure in Chemistry, 2022, 12, 141-157. | 1.8 | 9 |
| 15038 | A new organic-inorganic hybrid compound (NH ₃ (CH ₂)C ₆ H ₄ CO ₂ H)[SnCl ₆]: Synthesis, crystal structure, vibrational, optical, magnetic properties and theoretical study. Journal of Molecular Structure, 2021, 1234, 130129. | 2.1 | 4 |
| 15039 | Decomposed Mean-Field Simulations of Local Properties in Condensed Phases. Journal of Physical Chemistry Letters, 2021, 12, 6048-6055. | 1.2 | 0 |
| 15040 | Synthesis, photophysical properties, and computational studies of benzothiadiazole and/or phenothiazine based donor/acceptor π -conjugated copolymers. Journal of Polymer Research, 2021, 28, 1. | 3.2 | 48 |
| 15041 | Modulating Oxygen Reduction Behaviors on Nickel Single-Atom Catalysts to Probe the Electrochemiluminescence Mechanism at the Atomic Level. Analytical Chemistry, 2021, 93, 8663-8670. | 1.2 | 6 |
| 15042 | Electron binding energies and Dyson orbitals of OnH ₂ n+1+,0,â” clusters: Double Rydberg anions, Rydberg radicals, and micro-solvated hydronium cations. Journal of Chemical Physics, 2021, 154, 234304. | 1.6 | 4 |
| 15043 | Structural, Electronic, and Nonlinear Optical Properties of C ₆ H ₄ and C ₇ OCl ₆ Encapsulating Li and F Atoms. ACS Omega, 2021, 6, 16234-16240. | 2.5 | 8 |
| 15044 | Prediction of the Liquid-Liquid Extraction Properties of Imidazolium-Based Ionic Liquids for the Extraction of Aromatics from Aliphatics. Journal of Chemical Information and Modeling, 2021, 61, 3376-3385. | 1.7 | 6 |
| 15045 | Comparison of (5 + 2) Cycloadditions Involving Oxidopyrylium and Oxidopyridinium Ions: Relative Reactivities. Journal of Organic Chemistry, 2021, 86, 8652-8659. | 7.3 | 10 |
| 15046 | Electron-Induced Spin-Crossover in Self-Assembled Tetramers. ACS Nano, 2021, 15, 11770-11778. | 2.1 | 2 |
| 15047 | Fast Estimation of MÅller-Plesset Correlation Energies Based on Atomic Contributions. Journal of Physical Chemistry Letters, 2021, 12, 5324-5331. | 1.4 | 7 |
| 15048 | Solvent-Antisolvent Competitive Interactions Mediate Imidacloprid Polymorphs in Antisolvent Crystallization. Crystal Growth and Design, 2021, 21, 4318-4328. | 4.0 | 28 |
| 15049 | A Polymer-in-Salt Electrolyte with Enhanced Oxidative Stability for Lithium Metal Polymer Batteries. ACS Applied Materials & Interfaces, 2021, 13, 31583-31593. | 23.0 | 242 |
| 15050 | Fe(II) Redox Chemistry in the Environment. Chemical Reviews, 2021, 121, 8161-8233. | | |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15051 | How Accurate Are Approximate Density Functionals for Noncovalent Interaction of Very Large Molecular Systems?. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3967-3973. | 2.3 | 17 |
| 15052 | Thermochemical and kinetic studies of hydrogen abstraction reaction from C ₁₆ H ₁₀ isomers by H atoms. <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113257. | 1.1 | 4 |
| 15053 | Probing the origin of ambiphilic reactivity in osmapentayne complexes: Interplay of ring strain, aromaticity, and phosphonium substituent. <i>Journal of Organometallic Chemistry</i> , 2021, 945, 121866. | 0.8 | 1 |
| 15054 | First-principle kinetic studies of unimolecular pyrolysis of isopropyl esters as biodiesel surrogates. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1. | 0.5 | 8 |
| 15055 | Torsional Profiles of Thiophene and Furan Oligomers: Probing the Effects of Heterogeneity and Chain Length. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6228-6237. | 1.1 | 10 |
| 15056 | Adiabatic Molecular Orbital Tracking in Ab Initio Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4675-4685. | 2.3 | 3 |
| 15057 | Quercetin inhibits histamine-induced calcium influx in human keratinocyte via histamine H4 receptors. <i>International Immunopharmacology</i> , 2021, 96, 107620. | 1.7 | 12 |
| 15058 | Ni Oxidation State and Ligand Saturation Impact on the Capability of Octaazamacrocyclic Complexes to Bind and Reduce CO ₂ . <i>Molecules</i> , 2021, 26, 4139. | 1.7 | 3 |
| 15059 | Combined crossed molecular beams and computational study on the N(² D) + HCCCN(X ¹ Σ ⁺) reaction and implications for extra-terrestrial environments. <i>Molecular Physics</i> , 2022, 120, . | 0.8 | 9 |
| 15060 | Exact-two-component block-localized wave function: A simple scheme for the automatic computation of relativistic \hat{T}^2 SCF. <i>Journal of Chemical Physics</i> , 2021, 155, 014103. | 1.2 | 5 |
| 15061 | Bridging the 12-6-4 Model and the Fluctuating Charge Model. <i>Frontiers in Chemistry</i> , 2021, 9, 721960. | 1.8 | 4 |
| 15062 | New C ₂ - and N ₃ -Modified Thieno[2,3-d]Pyrimidine Conjugates with Cytotoxicity in the Nanomolar Range. <i>Anti-Cancer Agents in Medicinal Chemistry</i> , 2022, 22, 1201-1212. | 0.9 | 5 |
| 15063 | A Mechanistic Probe into 1,2- <i>cis</i> Glycoside Formation Catalyzed by Phenanthroline and Further Expansion of Scope. <i>Advanced Synthesis and Catalysis</i> , 2021, 363, 4054-4066. | 2.1 | 4 |
| 15064 | Ethoxylation of Phenols Catalyzed by σ -Metal-Free Lewis Pairs: Living/Controlled Polymerization in a σ -Slow-Initiation Mode. <i>Chinese Journal of Chemistry</i> , 2021, 39, 2579-2587. | 2.6 | 4 |
| 15065 | Synthesis, spectral, molecular modeling, biological and antitumor studies of new nifuroxazide complexes. <i>Materials Express</i> , 2021, 11, 1071-1083. | 0.2 | 0 |
| 15066 | Investigation of reactive properties, adsorption on fullerene, DFT, molecular dynamics simulation of an anthracene derivative targeting dihydrofolate reductase and human dUTPase. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-10. | 2.0 | 10 |
| 15067 | Pyramidal Dicationic Ge(II) Complexes with Homoleptic Neutral Prictine Coordination: A Combined Experimental and Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2021, 60, 12100-12108. | 1.9 | 6 |
| 15068 | A community-powered search of machine learning strategy space to find NMR property prediction models. <i>PLoS ONE</i> , 2021, 16, e0253612. | 1.1 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15069 | Acridone-amine D-A-D thermally activated delayed fluorescence emitters with narrow resolved electroluminescence and their electrochromic properties. <i>Electrochimica Acta</i> , 2021, 384, 138347. | 2.6 | 10 |
| 15070 | Combined Experimental and Theoretical Investigations on Structural, Spectroscopic, Electronic, and Nonlinear Optical Behaviour of Na ⁺ -(E)-(2,5-dimethoxyphenyl) methylidene]biphenyl-4-carbohydrazide Crystal. <i>ECS Journal of Solid State Science and Technology</i> , 2021, 10, 071008. | 0.9 | 0 |
| 15071 | Effectiveness of smearing and tetrahedron methods: best practices in DFT codes. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2021, 29, 065014. | 0.8 | 9 |
| 15072 | <i>syn</i> -Selective Construction of Fused Heterocycles by Catalytic Reductive Tandem Functionalization of N-Heteroarenes. <i>ACS Catalysis</i> , 2021, 11, 9271-9278. | 5.5 | 32 |
| 15073 | Chalcogen Bonds in Selenocysteine Seleninic Acid, a Functional GPx Constituent, and in Other Seleninic or Sulfinic Acid Derivatives. <i>Chemistry - an Asian Journal</i> , 2021, 16, 2351-2360. | 1.7 | 12 |
| 15074 | The Effect of Hartree-Fock Exchange on Scaling Relations and Reaction Energetics for C-H Activation Catalysts. <i>Topics in Catalysis</i> , 2022, 65, 296-311. | 1.3 | 11 |
| 15075 | The effect of ring aromaticity on ESIPT behavior and photophysical properties of 2-(2-hydroxyphenyl)-4-chloromethylthiazole derivatives: A TD-DFT study. <i>Journal of Molecular Liquids</i> , 2021, 334, 116517. | 2.3 | 15 |
| 15076 | Electronic Structure of Molecules, Surfaces, and Molecules on Surfaces with the Local Modified Becke-Johnson Exchange-Correlation Potential. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4746-4755. | 2.3 | 10 |
| 15077 | Electronic structure of mononuclear Cu-based molecule from density-functional theory with self-interaction correction. <i>Journal of Chemical Physics</i> , 2021, 155, 014106. | 1.2 | 12 |
| 15078 | Cationic Co(I) Catalysts for Regiodivergent Hydroalkenylation of 1,6-Enynes: An Uncommon <i>cis</i> -C-H Activation Leads to <i>Z</i> -Selective Coupling of Acrylates. <i>ACS Catalysis</i> , 2021, 11, 9605-9617. | 5.5 | 32 |
| 15079 | Computation of Solid-State Vibrational Circular Dichroism in the Periodic Gauge. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 7213-7220. | 2.1 | 23 |
| 15080 | Photoredox Catalytic Phosphate-Mediated Deoxygenation of β -Ketones Enables Wolff Rearrangement and Staudinger Synthesis of β -Lactams. <i>Angewandte Chemie</i> , 2021, 133, 19848-19852. | 1.6 | 2 |
| 15081 | Electronic Structure of Superoxidized Radical Cationic Dodecaborate-Based Clusters. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6141-6150. | 1.1 | 2 |
| 15082 | Machine learning based energy-free structure predictions of molecules, transition states, and solids. <i>Nature Communications</i> , 2021, 12, 4468. | 5.8 | 53 |
| 15083 | Second-Order Analytic Derivatives for XYG3 Type of Doubly Hybrid Density Functionals: Theory, Implementation, and Application to Harmonic and Anharmonic Vibrational Frequency Calculations. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4860-4871. | 2.3 | 7 |
| 15084 | Bi(III) halometallate ionic liquids: Interactions and speciation. <i>Journal of Chemical Physics</i> , 2021, 155, 014501. | 1.2 | 10 |
| 15085 | Electron-rich triarylphosphines as nucleophilic catalysts for oxa-Michael reactions. <i>Beilstein Journal of Organic Chemistry</i> , 2021, 17, 1689-1697. | 1.3 | 8 |
| 15086 | Bis(triazinyl)pyridine complexes of Pt(II) and Pd(II): studies of the nucleophilic substitution reactions, DNA/HSA interactions, molecular docking and biological activity. <i>Journal of Biological Inorganic Chemistry</i> , 2021, 26, 625-637. | 1.1 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15087 | Investigation of the reactivity properties of a thiourea derivative with anticancer activity by DFT and MD simulations. <i>Journal of Molecular Modeling</i> , 2021, 27, 217. | 0.8 | 21 |
| 15088 | 25-hydroxycholesterol interacts differently with lipids of the inner and outer membrane leaflet " The Langmuir monolayer study complemented with theoretical calculations. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2021, 211, 105909. | 1.2 | 9 |
| 15089 | Rotation about a Covalent Bond and Pyramidalization of an Adjacent sp ² Center are a Synchronized Molecular Motion. <i>Journal of Organic Chemistry</i> , 2021, 86, 10420-10426. | 1.7 | 3 |
| 15090 | Photoredox Catalytic Phosphite-Mediated Deoxygenation of β -Diketones Enables Wolff Rearrangement and Staudinger Synthesis of β -Lactams. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 19696-19700. | 7.2 | 19 |
| 15091 | Excited States of Xanthophylls Revisited: Toward the Simulation of Biologically Relevant Systems. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6604-6612. | 2.1 | 13 |
| 15092 | Impact of the Characteristics of Quantum Chemical Databases on Machine Learning Prediction of Tautomerization Energies. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4769-4785. | 2.3 | 12 |
| 15093 | First-principles correction scheme for linear-response time-dependent density functional theory calculations of core electronic states. <i>Journal of Chemical Physics</i> , 2021, 155, 034108. | 1.2 | 7 |
| 15094 | How Can the σ -Type Fullerene-Metal Bond Survive? A Systematic Survey of Reactions between Mono-EMFs and (M ²⁺ Ln) ² Dimers. <i>Inorganic Chemistry</i> , 2021, 60, 11287-11296. | 1.9 | 0 |
| 15095 | Symmetry-Binding Correlations of Crown Ether Complexes with Li ⁺ and Na ⁺ . <i>ACS Omega</i> , 2021, 6, 19233-19237. | 1.6 | 3 |
| 15096 | Testing Self-Interaction Correction for Molecules in Solution. <i>Advanced Engineering Materials</i> , 0, , 2100572. | 1.6 | 1 |
| 15097 | Density Functional Geometries and Zero-Point Energies in Ab Initio Thermochemical Treatments of Compounds with First-Row Atoms (H, C, N, O, F). <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4872-4890. | 2.3 | 22 |
| 15098 | Porphyrin dimer as efficient optical thermometer: Experimental and computational evaluation of the barrier to torsional rotation. <i>Journal of Luminescence</i> , 2021, 235, 117986. | 1.5 | 7 |
| 15099 | On the Low-Lying Electronically Excited States of Azobenzene Dimers: Transition Density Matrix Analysis. <i>Molecules</i> , 2021, 26, 4245. | 1.7 | 9 |
| 15100 | Excitonic characteristics of blue-emitting quantum dot materials in group II-VI using hybrid time-dependent density functional theory. <i>Physical Review B</i> , 2021, 104, . | 1.1 | 7 |
| 15101 | Benchmarking of Density Functionals for $\langle i \rangle Z \langle /i \rangle$ -Azoarene Half-Lives via Automated Transition State Search. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6474-6485. | 1.1 | 8 |
| 15102 | Chirality of the Conformation Attacks the Planarity of the sp ² Carbon Atom in a Covalent Bond. <i>Journal of Organic Chemistry</i> , 2021, 86, 10414-10419. | 1.7 | 2 |
| 15103 | Design, Synthesis and Characterization of Achiral Unsymmetrical Four-ring based Hockey-stick Shaped Liquid Crystals: Structure-Property relationship. <i>Liquid Crystals</i> , 2022, 49, 162-171. | 0.9 | 9 |
| 15104 | Mechanistic Insights into Iron-Catalyzed C-H Bond Activation and C-C Coupling. <i>Organometallics</i> , 2021, 40, 2467-2477. | 1.1 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15105 | How a crosslinker agent interacts with the β -glucosidase enzyme surface in an aqueous solution: Insight from quantum mechanics calculations and molecular dynamics simulations. <i>Colloids and Surfaces B: Biointerfaces</i> , 2021, 203, 111761. | 2.5 | 4 |
| 15106 | Structural studies of ligand stabilized Ni/Ga clusters by means of vibrational spectroscopy and theoretical calculations. <i>Journal of Raman Spectroscopy</i> , 2021, 52, 2317-2337. | 1.2 | 4 |
| 15107 | Nickel(II) complexes with 2-Hfur and N-donors: The magnetic effects of the structural variations, thermal properties and antimycobacterial activity against <i>Mycobacterium smegmatis</i> . <i>Polyhedron</i> , 2021, 203, 115241. | 1.0 | 19 |
| 15108 | The Beginning of HCN Polymerization: Iminoacetonitrile Formation and Its Implications in Astrochemical Environments. <i>ACS Earth and Space Chemistry</i> , 2021, 5, 2152-2159. | 1.2 | 13 |
| 15109 | Carbon-Based Hybrid Interlayer to Anchor the Shuttling of Polysulfides for High-Performance Lithium-Sulfur Batteries. <i>ACS Applied Energy Materials</i> , 2021, 4, 8294-8302. | 2.5 | 7 |
| 15110 | Relativistic corrections of the electric field gradient in dihalogen molecules XY (X, Y = F, Cl, Br, I, At) within the linear response elimination of the small component formalism. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26769. | 1.0 | 1 |
| 15111 | Doping alkali metal ions and introducing electron donor groups to fulleropyrrolidine derivatives: Large second-order nonlinear optical responses. <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113254. | 1.1 | 1 |
| 15112 | Theoretical Study on Understanding the Effects of Core Structure and Energy Level Tuning on Efficiency of Nonfullerene Acceptors in Organic Solar Cells. <i>Advanced Theory and Simulations</i> , 2021, 4, 2100019. | 1.3 | 5 |
| 15113 | Ab initio investigation on the low-lying states of La ₂ X ₂ (X = Se, Sn, Sb). <i>Canadian Journal of Physics</i> , 2021, 99, 735-740. | 0.4 | 1 |
| 15114 | Non-fullerene acceptor photostability and its impact on organic solar cell lifetime. <i>Cell Reports Physical Science</i> , 2021, 2, 100498. | 2.8 | 35 |
| 15115 | Pump-probe photoemission simulated in real time: Revealing many-particle signatures. <i>Physical Review A</i> , 2021, 104, . | 1.0 | 2 |
| 15116 | N-Heterocyclic Carbenes with a Nido-C ₂ B ₉ Carborane Backbone. <i>Chinese Journal of Chemistry</i> , 2021, 39, 2410-2416. | 2.6 | 7 |
| 15117 | Density-Based Many-Body Expansion as an Efficient and Accurate Quantum-Chemical Fragmentation Method: Application to Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4144-4156. | 2.3 | 13 |
| 15118 | iOI: An Iterative Orbital Interaction Approach for Solving the Self-Consistent Field Problem. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4831-4845. | 2.3 | 7 |
| 15119 | In-silico modelling of fullerene and fullerene adsorbed by nO ₂ molecules (n(O ₂)@C _m with n = 1, 2, 4). <i>Journal of Computational Chemistry</i> , 2021, 42, 1000000. | 0.8 | 4 |
| 15120 | Examination of How Well Long-Range-Corrected Density Functionals Satisfy the Ionization Energy Theorem. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4823-4830. | 2.3 | 17 |
| 15121 | Reaction Path-Force Matching in Collective Variables: Determining Ab Initio QM/MM Free Energy Profiles by Fitting Mean Force. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4961-4980. | 2.3 | 14 |
| 15122 | Theoretical investigation on conversion of CO ₂ with epoxides to cyclic carbonates by bifunctional metal-salen complexes bearing ionic liquid substituents. <i>Molecular Catalysis</i> , 2021, 511, 111733. | 1.0 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15123 | 3Å— Axial vs 3Å— Equatorial: The ρ^* Value Is a Robust Computational Measure of Substituent Steric Effects. <i>Journal of the American Chemical Society</i> , 2021, 143, 13573-13578. | 6.6 | 6 |
| 15124 | Structural (X-ray), spectroscopic (FT-IR, FT-Raman) and computational (DFT) analysis of intermolecular interactions in 1H-indazole-3-carbaldehyde. <i>Journal of Molecular Structure</i> , 2021, 1237, 130318. | 1.8 | 1 |
| 15125 | Isospecific alternating copolymerization of unprotected polar styrenes and ethylene by the C symmetric scandium precursor via synergistic effects of two substituent groups. <i>Giant</i> , 2021, 7, 100061. | 2.5 | 12 |
| 15126 | Intersystem Crossing in Boron-Based Donor-Spiro-Acceptor Organic Chromophore: A Detailed Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6674-6680. | 1.1 | 15 |
| 15127 | Synthesis, characterization, theoretical, and antimicrobial studies of indenoquinoxalin-based ligands and their reactions with CuBr(PPh ₃) ₃ . <i>Journal of Molecular Structure</i> , 2021, 1238, 130309. | 1.8 | 2 |
| 15128 | Distribution of H ^β Hyperfine Couplings in a Tyrosyl Radical Revealed by 263 GHz ENDOR Spectroscopy. <i>Applied Magnetic Resonance</i> , 2022, 53, 1015-1030. | 0.6 | 3 |
| 15129 | The inhibition performance of quinoa seed on corrosion behavior of carbon steel in the HCl solution; theoretical and experimental evaluations. <i>Journal of Molecular Liquids</i> , 2021, 335, 116183. | 2.3 | 26 |
| 15130 | Catalytic S _N Ar Hydroxylation and Alkoxylation of Aryl Fluorides. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 20391-20399. | 7.2 | 22 |
| 15131 | NAC-TDDFT: Time-Dependent Density Functional Theory for Nonadiabatic Couplings. <i>Accounts of Chemical Research</i> , 2021, 54, 3288-3297. | 7.6 | 17 |
| 15132 | Mechanism and Selectivities in Ru-Catalyzed Anti-Markovnikov Formal Hydroalkylation of 1,3-Dienes and Enynes: A Computational Study. <i>Journal of Organic Chemistry</i> , 2021, 86, 11895-11904. | 1.7 | 2 |
| 15133 | Heme-Heme Interactions in Diheme Cytochromes: Effect of Mixed-Axial Ligation on the Electronic Structure and Electrochemical Properties. <i>Inorganic Chemistry</i> , 2021, 60, 12870-12882. | 1.9 | 5 |
| 15134 | Solid-State Nuclear Magnetic Resonance Techniques for the Structural Characterization of Geminal Alane-Phosphane Frustrated Lewis Pairs and Secondary Adducts. <i>Chemistry - A European Journal</i> , 2021, 27, 13249-13257. | 1.7 | 4 |
| 15135 | Density Functional Theory for Electrocatalysis. <i>Energy and Environmental Materials</i> , 2022, 5, 157-185. | 7.3 | 95 |
| 15136 | Hydrogen Bonds and n-π* Interactions in the Acetylation of Propranolol Catalyzed by <i>Candida antarctica</i> Lipase B: A QAIM Study. <i>ACS Omega</i> , 2021, 6, 20992-21004. | 1.6 | 2 |
| 15137 | Functionally substituted arylhydrazones as building blocks in heterocyclic synthesis: Facile synthesis of pyrazoles, triazoles, triazines and quantum chemical studies. <i>Synthetic Communications</i> , 2021, 51, 3099-3115. | 1.1 | 2 |
| 15138 | Excited-state properties of Y-series small molecule semiconductors. <i>Dyes and Pigments</i> , 2021, 192, 109431. | 2.0 | 17 |
| 15139 | Development of Mg/Al/Si/O ReaxFF Parameters for Magnesium Aluminosilicate Glass Using an Artificial Neural Network-Assisted Genetic Algorithm. <i>Journal of Physical Chemistry C</i> , 2021, 125, 18380-18394. | 1.5 | 13 |
| 15140 | Revealing dissolution behavior of o-methoxybenzoic acid in twelve pure solvents using thermodynamic analysis and molecular simulation. <i>Journal of Molecular Liquids</i> , 2021, 336, 116242. | 2.3 | 15 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15141 | Reversible isomerization of metal nanoclusters induced by intermolecular interaction. <i>CheM</i> , 2021, 7, 2227-2244. | 5.8 | 38 |
| 15142 | Assemblies of Polyacrylonitrile-Derived Photoactive Polymers as Blue and Green Light Photo-Cocatalysts for Cu-Catalyzed ATRP in Water and Organic Solvents. <i>Frontiers in Chemistry</i> , 2021, 9, 734076. | 1.8 | 9 |
| 15143 | Local molecular probes of ultrafast relaxation channels in strongly coupled metalloporphyrin-cavity systems. <i>Journal of Chemical Physics</i> , 2021, 155, 064702. | 1.2 | 15 |
| 15144 | Identification of the structural features of quinazoline derivatives as EGFR inhibitors using 3D-QSAR modeling, molecular docking, molecular dynamics simulations and free energy calculations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 11125-11140. | 2.0 | 4 |
| 15145 | Quaternary ammonium salt functionalized MIL-101-NH ₂ (Cr) as a bifunctional catalyst for the cycloaddition of CO ₂ with epoxides to produce cyclic carbonates. <i>Applied Catalysis A: General</i> , 2021, 624, 118307. | 2.2 | 28 |
| 15146 | Bimetallic Platinum Group Complexes of a Macrocyclic Pyrazolate/NHC Hybrid Ligand. <i>Organometallics</i> , 2021, 40, 3056-3065. | 1.1 | 3 |
| 15147 | Synthesis, single crystal (XRD), Hirshfeld surface analysis, computational study (DFT) and molecular benzenesulfonamide. <i>Heliyon</i> , 2021, 7, e07724. | 1.4 | 51 |
| 15148 | The two redox states of the human NEET proteins TM [2Fe ²⁺ 2S] clusters. <i>Journal of Biological Inorganic Chemistry</i> , 2021, 26, 763-774. | 1.1 | 6 |
| 15149 | Catalytic Activity of Various β -diketiminato Zinc Complexes toward the Ring-Opening Polymerization of Caprolactone and Derivatives. <i>Macromolecular Chemistry and Physics</i> , 2021, 222, 2100187. | 1.1 | 6 |
| 15150 | A Simple Effective SCF Method for Computing Optical Gaps in Organic Chromophores. <i>Chemistry - an Asian Journal</i> , 2021, 16, 2729-2739. | 1.7 | 3 |
| 15151 | Structure and Absolute Configuration of Phenanthro-perylene Quinone Pigments from the Deep-Sea Crinoid <i>Hyalocrinus naresianus</i> . <i>Marine Drugs</i> , 2021, 19, 445. | 2.2 | 6 |
| 15152 | SAR11 Cells Rely on Enzyme Multifunctionality To Metabolize a Range of Polyamine Compounds. <i>MBio</i> , 2021, 12, e0109121. | 1.8 | 10 |
| 15153 | Density-functional theory studies of vanadium oxide clusters and their cations. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1. | 0.5 | 3 |
| 15154 | pH Effects and Cooperativity among Key Titratable Residues for <i>Escherichia coli</i> Glycinamide Ribonucleotide Transformylase. <i>Journal of Physical Chemistry B</i> , 2021, 125, 9168-9185. | 1.2 | 2 |
| 15155 | Spodium Bonds in Biological Systems: Expanding the Role of Zn in Protein Structure and Function. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3945-3954. | 2.5 | 21 |
| 15156 | DFT Study and Antiparasitic Activity of Some Azo Dyes Containing Uracil. <i>Journal of Chemistry</i> , 2021, 2021, 1-11. | 0.9 | 5 |
| 15157 | Citrulline malate transdermal delivery through integrating into polyvinyl alcohol (PVA) nanofibers. <i>Journal of Drug Delivery Science and Technology</i> , 2021, 64, 102630. | 1.4 | 3 |
| 15158 | Estimation of octanol-water partition coefficients of PCBs based on the solvation free energy. <i>Computational and Theoretical Chemistry</i> , 2021, 1202, 113324. | 1.1 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15159 | Photoisomerization of an Azobenzene-Containing Surfactant Within a Micelle. <i>ChemPhotoChem</i> , 2021, 5, 926-932. | 1.5 | 12 |
| 15160 | Additive and Emergent Catalytic Properties of Dimeric Unnatural Amino Acid Derivatives: Aldol and Conjugate Additions. <i>Chemistry - A European Journal</i> , 2021, 27, 15671-15687. | 1.7 | 5 |
| 15161 | Activator-free reactions of carboxylic ortho esters with cyclic 1,2-diketones. <i>Russian Chemical Bulletin</i> , 2021, 70, 1584-1598. | 0.4 | 1 |
| 15162 | Large-scale simulations of CO ₂ diffusion in metal-organic frameworks with open Cu sites. <i>Chinese Journal of Chemical Engineering</i> , 2022, 42, 1-9. | 1.7 | 3 |
| 15163 | Mild Open-Shell Character of BODIPY and Its Impact on Singlet and Triplet Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5825-5838. | 2.3 | 12 |
| 15164 | Unraveling the Mechanism of Aerobic Alcohol Oxidation by a Cu/pyridyl-1,2-Cyclodextrin/TEMPO Catalytic System under Air in Neat Water. <i>Inorganic Chemistry</i> , 2021, 60, 14132-14141. | 1.9 | 4 |
| 15165 | Extending π-Conjugation and Integrating Multiple Redox Centers into One Molecule for High-Capacity Organic Cathodes. <i>ChemSusChem</i> , 2021, 14, 3858-3866. | 3.6 | 17 |
| 15166 | Atmospheric Chemistry of 2-Amino-2-methyl-1-propanol: A Theoretical and Experimental Study of the OH-Initiated Degradation under Simulated Atmospheric Conditions. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7502-7519. | 1.1 | 5 |
| 15167 | Microbe-Assisted Nanocomposite Anodes for Aqueous Li-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 39195-39204. | 4.0 | 2 |
| 15168 | Temporary Anion Resonances of Pyrene: A 2D Photoelectron Imaging and Computational Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7004-7013. | 1.1 | 10 |
| 15169 | The proton sponge 1,8-bis(dimethylamino)naphthalene: The quicker-picker-upper also for s-block metal cations?. <i>Chemical Physics Letters</i> , 2021, 777, 138735. | 1.2 | 6 |
| 15170 | Elucidating the Impact of Mg Substitution on the Properties of NASICON (Na ₃ V ₂ P ₄ O ₁₄) Cathodes. <i>Advanced Functional Materials</i> , 2021, 31, 2105463. | 1.7 | 4 |
| 15171 | The Interplay between Diradical Character and Stability in Organic Molecules. <i>Symmetry</i> , 2021, 13, 1448. | 1.1 | 1 |
| 15172 | Fully relativistic study of polyatomic closed shell E121X3 (X = F, Cl, Br) molecules: effects of Gaunt interaction, relativistic effects and advantages of an exact-two component (X2C) hamiltonian. <i>Journal of Molecular Modeling</i> , 2021, 27, 262. | 0.8 | 1 |
| 15173 | Catalytic S _N Ar Hydroxylation and Alkoxylation of Aryl Fluorides. <i>Angewandte Chemie</i> , 2021, 133, 20554-20562. | 1.6 | 4 |
| 15174 | Ordering of Oxygen Vacancies and Related Ferroelectric Properties in HfO_2 . <i>Physical Review Letters</i> , 2021, 127, 087602. | 2.9 | 31 |
| 15175 | Langmuir-Blodgett Films of Diketopyrrolopyrroles with Tunable Amphiphilicity. <i>Langmuir</i> , 2021, 37, 10272-10278. | 1.6 | 3 |
| 15176 | Extrapolating DFT Toward the Complete Basis Set Limit: Lessons from the PBE Family of Functionals. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5651-5660. | 2.3 | 14 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 15177 | Identification of the Key Parameters for Horizontal Transition Dipole Orientation in Fluorescent and TADF Organic Light-Emitting Diodes. <i>Advanced Materials</i> , 2021, 33, e2100677. | 11.1 | 99 |
| 15178 | Accurate Heats of Formation for Polycyclic Aromatic Hydrocarbons: A High-Level Ab Initio Perspective. <i>Journal of Chemical & Engineering Data</i> , 2021, 66, 3453-3462. | 1.0 | 8 |
| 15179 | Efficient Approximation of Potential Energy Surfaces with Mixed-Basis Interpolation. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5673-5683. | 2.3 | 3 |
| 15180 | The effect of different substituent on ESIPT fluorescence features of 2-(2'-hydroxyphenyl)-4-chloro-methylthiazole derivatives: A DFT/TD-DFT study. <i>Chinese Physics B</i> , 0, , . | 0.7 | 0 |
| 15181 | Pyridine-containing octadentate ligand NE3TA-PY for formation of neutral complex with ¹⁷⁷ Lu(III) and ⁹⁰ Y(III) for radiopharmaceutical applications: Synthesis, DFT calculation, radiolabeling, and in vitro complex stability. <i>Journal of Inorganic Biochemistry</i> , 2021, 221, 111436. | 1.5 | 1 |
| 15182 | Ab initio and steady-state models for uranium isotope fractionation in multi-step biotic and abiotic reduction. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 307, 212-227. | 1.6 | 5 |
| 15183 | $\hat{x}^{\sim}[\text{Pd}(\text{dmit})_2]_2$ as a quasi-one-dimensional scalene Heisenberg model. <i>Physical Review Materials</i> , 2021, 5, . | 0.9 | 2 |
| 15184 | Tautomerism and basicity of carboxylic acid guanyl hydrazides (acylaminoguanidines). <i>Russian Chemical Bulletin</i> , 2021, 70, 1509-1522. | 0.4 | 2 |
| 15185 | Study of the Redox Potentials of Benzoquinone and Its Derivatives by Combining Electrochemistry and Computational Chemistry. <i>Journal of Chemical Education</i> , 2021, 98, 3019-3025. | 1.1 | 4 |
| 15186 | Review: materials and modelling for organic photovoltaic devices. <i>Polymer International</i> , 0, , . | 1.6 | 6 |
| 15187 | On assessing functional errors in density functional theory using atomisation energies and electric field gradients. <i>International Journal of Quantum Chemistry</i> , 0, , e26799. | 1.0 | 1 |
| 15188 | Highly selective and sensitive chiral recognition to deoxynucleosides by calixarene oligomers modified silver nanoparticles. <i>Sensors and Actuators B: Chemical</i> , 2021, 341, 130044. | 4.0 | 6 |
| 15189 | Visible-light-driven photoelectrocatalytic degradation of p-chloronitrobenzene by BiOBr/TiO ₂ nanotube arrays photoelectrodes: Mechanisms, degradation pathway and DFT calculation. <i>Separation and Purification Technology</i> , 2021, 268, 118699. | 3.9 | 28 |
| 15190 | Viologen-Decorated TEMPO for Neutral Aqueous Organic Redox Flow Batteries. <i>Energy Material Advances</i> , 2021, 2021, . | 4.7 | 29 |
| 15191 | Accurate Thermochemistry for Main-Group Elements up to Xenon with the W _n -P34 Series of Composite Methods. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5704-5714. | 2.3 | 14 |
| 15192 | Deep eutectic solvents with multiple weak acid sites for highly efficient, reversible and selective absorption of ammonia. <i>Separation and Purification Technology</i> , 2021, 269, 118791. | 3.9 | 42 |
| 15193 | Accurate fragment-based 51-V chemical shift predictions in molecular crystals. <i>Solid State Nuclear Magnetic Resonance</i> , 2021, 114, 101733. | 1.5 | 3 |
| 15194 | Implicit solvation in domain based pair natural orbital coupled cluster (DLPNO-CCSD) theory. <i>Journal of Computational Chemistry</i> , 2021, 42, 1959-1973. | 1.5 | 11 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15195 | Predictive optical photoabsorption of Ag ₂₄ Au(DMBT) ₁₈ via efficient TDDFT simulations. Journal of Chemical Physics, 2021, 155, 084103. | 1.2 | 12 |
| 15196 | Surface-enhanced Raman scattering of thiram: Quantitative and theoretical analyses. Journal of Raman Spectroscopy, 2021, 52, 2557-2571. | 1.2 | 23 |
| 15197 | Ylide-Substituted Phosphines with a Cyclic Ylide-Backbone: Angle Dependence of the Donor Strength. Organometallics, 2021, 40, 2888-2900. | 1.1 | 11 |
| 15198 | Polyacetylene Revisited: A Computational Study of the Molecular Engineering of N-type Polyacetylene. Journal of Physical Chemistry Letters, 2021, 12, 7745-7751. | 2.1 | 2 |
| 15199 | An excited state coupled-cluster study on indigo dyes. Molecular Physics, 0, , e1965235. | 0.8 | 8 |
| 15200 | Applications of Density Functional Theory on Heavy Metal Sensor and Hydrogen Evolution Reaction (HER). , 0, , . | | 0 |
| 15201 | Maximizing TADF via Conformational Optimization. Journal of Physical Chemistry A, 2021, 125, 7644-7654. | 1.1 | 11 |
| 15202 | Machine Learning Directed Optimization of Classical Molecular Modeling Force Fields. Journal of Chemical Information and Modeling, 2021, 61, 4400-4414. | 2.5 | 29 |
| 15203 | Assessment of DFT methods for the prediction of detachment energies and electronic structures of complex and multiply charged anions. Computational and Theoretical Chemistry, 2021, 1202, 113295. | 1.1 | 4 |
| 15204 | Significant increase in dipole moments of functional groups using cation bonding for excellent SERS sensing as a universal approach. Sensors and Actuators B: Chemical, 2021, 340, 129960. | 4.0 | 8 |
| 15205 | Photomediated ring contraction of saturated heterocycles. Science, 2021, 373, 1004-1012. | 6.0 | 58 |
| 15206 | Negatively charged polymeric interphase for regulated uniform lithium-ion transport in stable lithium metal batteries. Nano Energy, 2021, 87, 106214. | 8.2 | 18 |
| 15207 | Electronic <i>g</i> -Tensor Calculations for Dangling Bonds in Nanodiamonds. Journal of Physical Chemistry A, 2021, 125, 8249-8260. | 1.1 | 2 |
| 15208 | Fundamentals of Density Functional Theory: Recent Developments, Challenges and Future Horizons. , 0, , . | | 5 |
| 15209 | Black Phosphorene Modified Electrochemical Sensor for Fast Determination of 5-Hydroxymethyl-2-furfural in Milk. Electroanalysis, 2021, 33, 2452-2459. | 1.5 | 7 |
| 15210 | Structure and Thermodynamics of Eu(III) and Cm(III) Complexes with Glucuronic Acid. Inorganic Chemistry, 2021, 60, 14667-14678. | 1.9 | 1 |
| 15211 | Time-Resolved Spectroscopy and Electronic Structure of Mono- and Dinuclear Pyridyl-Triazole/DPEPhos-Based Cu(I) Complexes. Chemistry - A European Journal, 2021, 27, 15252-15271. | 1.7 | 14 |
| 15212 | Synergistic desulfurization over graphitic N and enzyme-like Fe-N sites of Fe-N-C. Chemical Engineering Journal, 2022, 430, 132657. | 6.6 | 20 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15213 | A self-consistent systematic optimisation of range-separated hybrid functionals from first principles. <i>Molecular Physics</i> , 0, , . | 0.8 | 3 |
| 15214 | Using Two Compatible Donor Polymers Boosts the Efficiency of Ternary Organic Solar Cells to 17.7%. <i>Chemistry of Materials</i> , 2021, 33, 7254-7262. | 3.2 | 35 |
| 15215 | A Structural Diversity of Molecular Alkaline-Earth-Metal Polyphosphides: From Supramolecular Wheel to Zintl Ion. <i>Chemistry - A European Journal</i> , 2021, 27, 14128-14137. | 1.7 | 6 |
| 15216 | Spectroscopically Guided Simulations Reveal Distinct Strategies for Positioning Substrates to Achieve Selectivity in Nonheme Fe(II)/ β -Ketoglutarate-Dependent Halogenases. <i>ACS Catalysis</i> , 2021, 11, 12394-12408. | 5.5 | 20 |
| 15217 | Accurate H-atom parameters for the two polymorphs of α -histidine at 5, 105 and 295 K. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 785-800. | 0.5 | 3 |
| 15219 | Raman spectroscopy signatures for monomeric, dimeric and trimeric zinc dimethoxide with tetrahydrofuran adduct and early hydrolysis-condensation products on Au(111) surface: theoretical and experimental approach. <i>Journal of Sol-Gel Science and Technology</i> , 2022, 102, 160-171. | 1.1 | 1 |
| 15220 | Mechanistic study on the photo carboxylation of benzylic C-H bonds by xanthone and Ni(0) catalysts. <i>Molecular Catalysis</i> , 2021, 514, 111785. | 1.0 | 3 |
| 15221 | Efficient access to aliphatic esters by photocatalyzed alkoxycarbonylation of alkenes with alkyloxalyl chlorides. <i>Nature Communications</i> , 2021, 12, 5328. | 5.8 | 36 |
| 15222 | A Comprehensive Experimental and Kinetic Modeling Study of the Combustion Chemistry of Diethoxymethane. <i>Energy & Fuels</i> , 2021, 35, 16086-16100. | 2.5 | 11 |
| 15223 | The Reactivity of Human and Equine Estrogen Quinones towards Purine Nucleosides. <i>Symmetry</i> , 2021, 13, 1641. | 1.1 | 0 |
| 15224 | Regularities of the property changes in the compounds EuLnCuS_3 (Ln = La-Lu). <i>Journal of Alloys and Compounds</i> , 2021, 874, 159968. | 2.8 | 13 |
| 15225 | Effects of functionalization of Y6 end-groups with electron-withdrawing groups on the photovoltaic properties at the donor-acceptor interfaces of PM6/Y6 OSCs: A theoretical insight. <i>Organic Electronics</i> , 2021, 96, 106235. | 1.4 | 12 |
| 15226 | Towards highly accurate calculations of parity violation in chiral molecules: relativistic coupled-cluster theory including QED-effects. <i>Molecular Physics</i> , 2021, 119, . | 0.8 | 13 |
| 15227 | Reduced-gradient analysis of van der Waals complexes. <i>Electronic Structure</i> , 2021, 3, 034009. | 1.0 | 7 |
| 15228 | Mechanism of reactivation of the peroxidase catalytic activity of human cyclooxygenases by reducing cosubstrate quercetin. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 107, 107941. | 1.3 | 6 |
| 15229 | Molecular dynamics simulations of quinine encapsulation into biodegradable nanoparticles: A possible new strategy against Sars-CoV-2. <i>European Polymer Journal</i> , 2021, 158, 110685. | 2.6 | 15 |
| 15230 | Mapping the Origins of Surface- and Chemistry-Dependent Doping Trends in In_2S_3 Quantum Dots with Density Functional Theory. <i>Chemistry of Materials</i> , 2021, 33, 7113-7123. | 3.2 | 6 |
| 15231 | Computational Mechanistic Study of Fused Phenol Formations from 1,6-Heptadiyne Involving Carbyne Complexes. <i>ChemCatChem</i> , 0, , . | 1.8 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15232 | Theoretical Insight into 20â€Electron Transition Metal Complexes (C ₅ H ₅) ₂ TM(E ₁ E ₂) ₂ (TM = Cr, Tj, Er, Yb, Lu, Sc, Ti, Zr, Hf, Nb, Ta, Mo, W, Re, Os, Ir, Pt, Au, Hg, Pb, Bi, Po, At, Rn). Bonding Nature. <i>Physica Status Solidi (B): Basic Research</i> , 2021, 258, 2100417. | 0.7 | 0 |
| 15233 | Lewis Acidâ€Promoted Oxidative Addition at a [Ni ⁰ (diphosphine) ₂] Complex: The Critical Role of a Secondary Coordination Sphere. <i>Chemistry - A European Journal</i> , 2021, 27, 16021-16027. | 1.7 | 16 |
| 15234 | Helical Covalent Polymers with Unidirectional Ion Channels as Single Lithium-Ion Conducting Electrolytes. <i>CCS Chemistry</i> , 2021, 3, 2762-2770. | 4.6 | 23 |
| 15235 | Assessment of the Accuracy of Density Functionals for Calculating Oxygen Reduction Reaction on Nitrogen-Doped Graphene. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6405-6415. | 2.3 | 9 |
| 15236 | Reaction mechanisms involving peroxy radical in the low-temperature oxidation of coal. <i>Fuel</i> , 2021, 300, 120943. | 3.4 | 31 |
| 15237 | A Comprehensive Picture of the Structures, Energies, and Bonding in the Alanine Dimers. <i>ChemPhysChem</i> , 2021, 22, 2401-2412. | 1.0 | 7 |
| 15238 | Oriented External Electric Field Tuning of Unsubstituted Azoheteroarene Thermal Isomerization Half-Lives. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8238-8248. | 1.1 | 2 |
| 15239 | Dendritic Iron(III) Carbazole Complexes: Structural, Optical, and Magnetic Characteristics. <i>Materials</i> , 2021, 14, 5445. | 1.3 | 7 |
| 15240 | A theoretical mechanistic study of [Kâ€Sâ€][2.2.2] ⁺ enantiomerization. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, e4289. | 0.9 | 2 |
| 15241 | Crystal Structure and Solid-State Packing of 4-Chloro-5H-1,2,3-dithiazol-5-one and 4-Chloro-5H-1,2,3-dithiazole-5-thione. <i>Molecules</i> , 2021, 26, 5875. | 1.7 | 3 |
| 15242 | Spectroscopic glimpses of the transition state of ATP hydrolysis trapped in a bacterial DnaB helicase. <i>Nature Communications</i> , 2021, 12, 5293. | 5.8 | 13 |
| 15243 | Investigation of Pharmaceutical Importance of 2H-Pyran-2-One Analogues via Computational Approaches. <i>Symmetry</i> , 2021, 13, 1619. | 1.1 | 2 |
| 15244 | Phosphine Evaluation on a New Series of Heteroleptic Copper(I) Photocatalysts with dpa Ligand [Cu(dpa)(P ₄)]BF ₄ . <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 4020-4029. | 1.0 | 12 |
| 15245 | Mono- and tetranuclear Fe(II,III) complexes with primary 1,3-diaminopropane: Synthetic aspects, magnetic properties and thermal behavior. <i>Polyhedron</i> , 2021, 206, 115354. | 1.0 | 2 |
| 15246 | A Convenient DFT-Based Strategy for Predicting Transition Temperatures of Valence Tautomeric Molecular Switches. <i>Inorganic Chemistry</i> , 2021, 60, 14475-14487. | 1.9 | 14 |
| 15247 | Modulation of the Activity and Regioselectivity of a Glycosidase: Development of a Convenient Tool for the Synthesis of Specific Disaccharides. <i>Molecules</i> , 2021, 26, 5445. | 1.7 | 0 |
| 15248 | Benzothiazole- vs. pyrazole-based unsymmetrical (PCN) pincer complexes of nickel(II) as homogeneous catalysts in ethylene oligomerization. <i>Journal of Organometallic Chemistry</i> , 2021, 949, 121951. | 0.8 | 10 |
| 15249 | Kojic acid derivatives as double face ligands for metal and phosphate ions.. <i>Journal of Inorganic Biochemistry</i> , 2021, 222, 111520. | 1.5 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15250 | Novel c-Jun N-Terminal Kinase (JNK) Inhibitors with an 11H-Indeno[1,2-b]quinoxalin-11-one Scaffold. <i>Molecules</i> , 2021, 26, 5688. | 1.7 | 11 |
| 15251 | Computing molecular excited states on a D-Wave quantum annealer. <i>Scientific Reports</i> , 2021, 11, 18796. | 1.6 | 16 |
| 15252 | Molecular modelling of two coordination states of Zn(II) ion at the active site of human carbonic anhydrase II. <i>Chemical Physics</i> , 2021, 549, 111281. | 0.9 | 3 |
| 15253 | <i>In Silico</i> study of Rosmarinic Acid Derivatives as Novel Insulin Fibril Inhibitors. <i>Journal of Computational Biophysics and Chemistry</i> , 2021, 20, 641-654. | 1.0 | 2 |
| 15254 | Ultrafast Dynamics and Estimation of Singlet Exciton Diffusion Parameters for Nanoaggregates of <i>peri</i> and <i>bay</i> Anisyl Perylene. <i>Journal of Physical Chemistry C</i> , 2021, 125, 20405-20415. | 1.5 | 4 |
| 15255 | Computational Study of Benzosultam Formation through Gold(I)-Catalyzed Ammoniumation/Nucleophilic Substitution Reaction. <i>Helvetica Chimica Acta</i> , 2021, 104, e2100133. | 1.0 | 3 |
| 15256 | Application of density functional theory on the NO-char heterogeneous reduction mechanism in the presence of CO ₂ . <i>Journal of Fuel Chemistry and Technology</i> , 2021, 49, 1231-1238. | 0.9 | 1 |
| 15257 | Surprisingly Good Performance of XYG3 Family Functionals Using a Scaled KS-MP3 Correlation. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9368-9376. | 2.1 | 7 |
| 15258 | A CDFT-Based Computational Peptidology (CDFT-CP) Study of the Chemical Reactivity and Bioactivity of the Marine-Derived Alternaramide Cyclopentadepsipeptide. <i>Journal of Chemistry</i> , 2021, 2021, 1-11. | 0.9 | 3 |
| 15259 | Computational study of bridge-splitting, aryl halide oxidative addition to PtII, and reductive elimination from PtIV: a route to pincer-PtII reagents with chemical and biological applications. <i>Chemistry - A European Journal</i> , 2021, 27, 15426-15433. | 1.7 | 0 |
| 15260 | Structural, antioxidant, antiproliferative and <i>in silico</i> study of pyridine-based hydrazone-selenazoles and their sulphur isosteres. <i>Journal of Molecular Structure</i> , 2021, 1240, 130512. | 1.8 | 18 |
| 15261 | Study on Chemical Bond Dissociation and the Removal of Oxygen-Containing Functional Groups of Low-Rank Coal during Hydrothermal Carbonization: DFT Calculations. <i>ACS Omega</i> , 2021, 6, 25772-25781. | 1.6 | 3 |
| 15262 | Supramolecular Reorientation During Deposition Onto Metal Surfaces of Quasi-Two-Dimensional Langmuir Monolayers Composed of Bifunctional Amphiphilic, Twisted Perylenes. <i>Langmuir</i> , 2021, 37, 11018-11026. | 1.6 | 8 |
| 15263 | Machine Learning-Assisted Selection of Active Spaces for Strongly Correlated Transition Metal Systems. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6053-6072. | 2.3 | 17 |
| 15264 | Chemically Modified Quinoidal Oligothiophenes for Enhanced Linear and Third-Order Nonlinear Optical Properties. <i>ACS Omega</i> , 2021, 6, 24602-24613. | 1.6 | 31 |
| 15265 | Systematical study on electronic properties of monoazaphenanthrene compounds. <i>Chemical Physics</i> , 2021, 552, 111370. | 0.9 | 0 |
| 15266 | A trinuclear copper (II) complex of naproxen-appended salicylhydrazide: Synthesis, crystal structure, DNA binding and molecular docking study. <i>Applied Organometallic Chemistry</i> , 0, , e6459. | 1.7 | 3 |
| 15267 | Using general computational chemistry strategy to unravel the reactivity of emerging pollutants: An example of sulfonamide chlorination. <i>Water Research</i> , 2021, 202, 117391. | 5.3 | 13 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15268 | Toward the Practical Use of Cobalt-Free Lithium-Ion Batteries by an Advanced Ether-Based Electrolyte. ACS Applied Materials & Interfaces, 2021, 13, 44339-44347. | 4.0 | 24 |
| 15269 | Extraction of Noncondensed Lignin from Poplar Sawdusts with <i>p</i> -Toluenesulfonic Acid and Ethanol. Journal of Agricultural and Food Chemistry, 2021, 69, 10838-10847. | 2.4 | 20 |
| 15270 | Prediction of Partition Coefficients in SDS Micelles by DFT Calculations. Symmetry, 2021, 13, 1750. | 1.1 | 3 |
| 15271 | Interaction of propionate and ethylamine on kagome phosphorene nanoribbons – A DFT study. Chemical Physics, 2021, 549, 111276. | 0.9 | 16 |
| 15272 | Core-Valence Attosecond Transient Absorption Spectroscopy of Polyatomic Molecules. Physical Review Letters, 2021, 127, 123001. | 2.9 | 18 |
| 15273 | Proposal of a Fermi–Dirac-Derived Reactivity Descriptor: Beyond the Frontier MO Model. Journal of Physical Chemistry A, 2021, 125, 8090-8097. | 1.1 | 2 |
| 15274 | Quantitative Estimation of the Hydrogen-Atom-Donating Ability of 4-Substituted Hantzsch Ester Radical Cations. ACS Omega, 2021, 6, 23621-23629. | 1.6 | 11 |
| 15275 | Mechanisms behind high CO ₂ /CH ₄ selectivity using ZIF-8 metal organic frameworks with encapsulated ionic liquids: A computational study. Chemical Engineering Journal, 2021, 419, 129638. | 6.6 | 19 |
| 15276 | Multicolor Phenylenediamine Carbon Dots for Metal-Ion Detection with Picomolar Sensitivity. ACS Applied Nano Materials, 2021, 4, 9919-9931. | 2.4 | 31 |
| 15277 | Artificial Intelligence Designer for Highly-Efficient Organic Photovoltaic Materials. Journal of Physical Chemistry Letters, 2021, 12, 8847-8854. | 2.1 | 15 |
| 15278 | Spatial Contributions to ¹ H NMR Chemical Shifts of Free-Base Porphyrinoids. Chemistry, 2021, 3, 1005-1021. | 0.9 | 6 |
| 15279 | Kinetic analysis of the effect of O ₂ on SF ₆ over-thermal decomposition. Journal Physics D: Applied Physics, 2021, 54, 495502. | 1.3 | 12 |
| 15280 | Structural, surface, and computational analysis of two vitamin-B1 crystals with sulfonimide-based anions. Zeitschrift Fur Kristallographie - Crystalline Materials, 2021, . | 0.4 | 0 |
| 15281 | Structural Dynamics of C ₂ F ₄ I ₂ in Cyclohexane Studied via Time-Resolved X-ray Liquidography. International Journal of Molecular Sciences, 2021, 22, 9793. | 1.8 | 4 |
| 15282 | Strong dependence on multistructural anharmonicity of the relative rates of intramolecular H-migration in alkylperoxyl and methylcyclohexylperoxyl radicals. Combustion and Flame, 2021, 231, 111503. | 2.8 | 6 |
| 15283 | Theoretical Prediction and Interpretation of ²³⁷ Np Mössbauer Isomer Shifts. Journal of Chemical Theory and Computation, 2021, 17, 6166-6179. | 2.3 | 3 |
| 15284 | Are Heavy Pnictogen–C Interactions Really –C Interactions?. Chemistry - A European Journal, 2021, 27, 14520-14526. | 1.7 | 5 |
| 15285 | The Catalytic Mechanism of the Retaining Glycosyltransferase Mannosylglycerate Synthase. Chemistry - A European Journal, 2021, 27, 13998-14006. | 1.7 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15286 | How Aromatic Fluorination Exchanges the Interaction Role of Pyridine with Carbonyl Compounds: The Formaldehyde Adduct. <i>Chemistry - A European Journal</i> , 2021, 27, 13870-13878. | 1.7 | 6 |
| 15287 | Structural, theoretical and enzyme-like activities of novel Cu(II) and Mn(II) complexes with coumarin based bidentate ligand. <i>Inorganica Chimica Acta</i> , 2021, 524, 120430. | 1.2 | 9 |
| 15288 | Absorption performance and reaction mechanism study on a novel anhydrous phase change absorbent for CO ₂ capture. <i>Chemical Engineering Journal</i> , 2021, 420, 129897. | 6.6 | 27 |
| 15289 | Ultra-stable anti-counterfeiting materials inspired by water stains. <i>Cell Reports Physical Science</i> , 2021, 2, 100571. | 2.8 | 8 |
| 15290 | Understanding Water-Zeolite Interactions: On the Accuracy of Density Functionals. <i>Journal of Physical Chemistry C</i> , 2021, 125, 20261-20274. | 1.5 | 10 |
| 15291 | Synthesis of selenophene substituted benzodithiophene and fluorinated benzothiadiazole based conjugated polymers for organic solar cell applications. <i>Electrochimica Acta</i> , 2021, 398, 139298. | 2.6 | 8 |
| 15292 | The origin of conformational solvatochromism in phenylmethylidene-bis(pyrrolo[2,3-b]quinoxaline) derivative. <i>Dyes and Pigments</i> , 2021, 193, 109475. | 2.0 | 0 |
| 15293 | Combinations of density functionals for accurate molecular properties of Be/W/H compounds. <i>Nuclear Materials and Energy</i> , 2021, 28, 101026. | 0.6 | 0 |
| 15294 | Studies on molecular mechanism between SHP2 and pyridine derivatives by 3D-QSAR, molecular docking and MD simulations. <i>Journal of Saudi Chemical Society</i> , 2021, 25, 101346. | 2.4 | 4 |
| 15295 | Ionic Functionalization of Multivariate Covalent Organic Frameworks to Achieve an Exceptionally High Iodine-Capture Capacity. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 22432-22440. | 7.2 | 148 |
| 15296 | Ionic Functionalization of Multivariate Covalent Organic Frameworks to Achieve an Exceptionally High Iodine-Capture Capacity. <i>Angewandte Chemie</i> , 2021, 133, 22606-22614. | 1.6 | 9 |
| 15297 | Origin of Increased Reactivity in Rhenium-Mediated Cycloadditions of Tetrazines. <i>Journal of Organic Chemistry</i> , 2021, 86, 13129-13133. | 1.7 | 11 |
| 15298 | The role of electric field on decomposition of CL-HMX cocrystal: A reactive molecular dynamics study. <i>Journal of Computational Chemistry</i> , 2021, 42, 2202-2212. | 1.5 | 8 |
| 15299 | Equation of motion coupled-cluster study of core excitation spectra II: Beyond the dipole approximation. <i>Journal of Chemical Physics</i> , 2021, 155, 094103. | 1.2 | 15 |
| 15300 | Machine Learning Approach for Describing Water OH Stretch Vibrations. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6353-6365. | 2.3 | 7 |
| 15301 | Chelate Coordination Compounds as a New Class of High-Energy Materials: The Case of Nitro-Bis(Acetylacetonato) Complexes. <i>Molecules</i> , 2021, 26, 5438. | 1.7 | 2 |
| 15302 | Machine Learning to Predict Diels-Alder Reaction Barriers from the Reactant State Electron Density. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6203-6213. | 2.3 | 16 |
| 15304 | Cracking and Dehydrogenation of Cyclohexane by [(phen)M(X)] ⁺ (M = Ni, Pd, Pt; X = H.) <i>Tj ETQq1 1 0,784314 rgBT /Over</i> | 1.1 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15305 | Interactions of Cellulose Model Compound Dâ€Cellobiose with Selected Metal Chlorides in Water: Identification of Chelating Oxygen Atoms. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 4968-4973. | 1.2 | 2 |
| 15306 | Ortho-Deuteration of Aromatic Aldehydes via a Transient Directing Group-Enabled Pd-Catalyzed Hydrogen Isotope Exchange. <i>Journal of Organic Chemistry</i> , 2021, 86, 13350-13359. | 1.7 | 10 |
| 15307 | De Novo Simulation of Charge Transport through Organic Single-Carrier Devices. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6416-6422. | 2.3 | 5 |
| 15308 | Quantum chemical exploration on the inhibition performance of indole and some of its derivatives against copper corrosion. <i>Journal of Molecular Liquids</i> , 2021, 340, 117136. | 2.3 | 11 |
| 15309 | Interacting Quantum Atoms Method for Crystalline Solids. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9011-9025. | 1.1 | 7 |
| 15310 | Internment of polysulfide in fractal carbon structure for high rate lithium-sulfur batteries. <i>Applied Surface Science</i> , 2021, 564, 150294. | 3.1 | 12 |
| 15311 | Novel sterically demanding Schiff base dyes: An insight from experimental and theoretical calculations. <i>Journal of Luminescence</i> , 2021, 238, 118264. | 1.5 | 12 |
| 15312 | Density functional theory investigation of the electronic and optical properties of metallo-phthalocyanine derivatives. <i>Optical Materials</i> , 2021, 120, 111315. | 1.7 | 10 |
| 15313 | Exploring the interaction of quercetin-3-O-sophoroside with SARS-CoV-2 main proteins by theoretical studies: A probable prelude to control some variants of coronavirus including Delta. <i>Arabian Journal of Chemistry</i> , 2021, 14, 103353. | 2.3 | 4 |
| 15314 | Theoretical exploration of optoelectronic performance of PM6:Y6 series-based organic solar cells. <i>Surfaces and Interfaces</i> , 2021, 26, 101385. | 1.5 | 15 |
| 15315 | Synthesis, crystal structure, IR spectroscopy, and DFT computation of the new variety of 2-carboxyanilinium dihydrogen phosphate (C ₇ H ₈ NO ₂ ⁺ . H ₂ PO ₄ ⁻). <i>Journal of Molecular Structure</i> , 2021, 1242, 130707. | 1.8 | 1 |
| 15316 | Shapeshifting radicals. <i>Chemical Physics</i> , 2022, 552, 111373. | 0.9 | 1 |
| 15317 | Demystifying the Origin of Vibrational Coherence Transfer Between the S ₁ and T ₁ States of the Pt-pop Complex. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9768-9773. | 2.1 | 6 |
| 15318 | Oxidation mechanism of ammonia in water clusters. <i>Molecular Physics</i> , 0, , . | 0.8 | 0 |
| 15319 | Pentaphosphaferrocene-mediated synthesis of asymmetric organo-phosphines starting from white phosphorus. <i>Nature Communications</i> , 2021, 12, 5774. | 5.8 | 31 |
| 15320 | A comparative study based on activity, conformation and computational analysis on the inhibition of human salivary aldehyde dehydrogenase by phthalate plasticizers: Implications in assessing the safety of packaged food items. <i>Toxicology</i> , 2021, 462, 152947. | 2.0 | 19 |
| 15321 | Efficient enantioresolution of aromatic $\hat{\pm}$ -hydroxy acids with Cinchona alkaloid-based zwitterionic stationary phases and volatile polar-ionic eluents. <i>Analytica Chimica Acta</i> , 2021, 1180, 338928. | 2.6 | 8 |
| 15322 | First-principles characterisation of spectroscopic and bonding properties of cationic bismuth carbide clusters. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113372. | 1.1 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15323 | Decavanadate salts of piperidine and triethanolamine: A combined experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2021, 1241, 130677. | 1.8 | 2 |
| 15324 | Unknown Knowns: Case studies in uncertainties in the computation of thermochemical parameters. <i>Chemical Physics</i> , 2021, 550, 111251. | 0.9 | 0 |
| 15325 | Effects of hydrophobic solute on water normal modes. <i>Chemical Physics</i> , 2021, 550, 111303. | 0.9 | 2 |
| 15326 | CAT-COSMO-CAMPD: Integrated in silico design of catalysts and processes based on quantum chemistry. <i>Computers and Chemical Engineering</i> , 2021, 153, 107438. | 2.0 | 6 |
| 15327 | Molecular and electronic structures of two new Schiff base compounds: (E)-2-bromo-6-[(2-bromo-4-methylphenylimino) methyl]-4-chlorophenol and (E)-2-bromo-6-[(4-bromo-3-methylphenylimino) methyl]-4-chlorophenol. <i>Journal of Molecular Structure</i> , 2021, 1241, 130643. | 1.8 | 2 |
| 15328 | Peroxymonosulfate activation through 2D/2D Z-scheme CoAl-LDH/BiOBr photocatalyst under visible light for ciprofloxacin degradation. <i>Journal of Hazardous Materials</i> , 2021, 420, 126613. | 6.5 | 150 |
| 15329 | Assessment of density functional theory in studying on the transition states of a Diiron-mediated N N bond cleavage reaction. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113418. | 1.1 | 1 |
| 15330 | Synthesis, structural investigation, computational study, antimicrobial activity and molecular docking studies of novel synthesized (E)-4-((pyridine-4-ylmethylene)amino)-N-(pyrimidin-2-yl)benzenesulfonamide from pyridine-4-carboxaldehyde and sulfadiazine. <i>Journal of Molecular Structure</i> , 2021, 1241, 130544. | 1.8 | 55 |
| 15331 | Adsorption of alkali and alkaline earth ions on nanocages using density functional theory. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113391. | 1.1 | 35 |
| 15332 | Unveiling the photophysical, biomolecule binding and photo-oxidative capacity of novel Ru(II)-polypyridyl corroles: A multipronged approach. <i>Journal of Molecular Liquids</i> , 2021, 340, 117223. | 2.3 | 10 |
| 15333 | Realizing wide-temperature Zn metal anodes through concurrent interface stability regulation and solvation structure modulation. <i>Energy Storage Materials</i> , 2021, 42, 517-525. | 9.5 | 47 |
| 15334 | Sub-zero and room-temperature sodium-sulfur battery cell operations: A rational current collector, catalyst and sulphur-host design and study. <i>Energy Storage Materials</i> , 2021, 42, 608-617. | 9.5 | 14 |
| 15335 | A critical evaluation of $[ML(ONO)]^+$ ($M = Fe, Ru, Os$) as nitric oxide precursor influenced by spin multiplicity and geometrical parameters (M-O-NO and MO-N-O) for the NO release: A theoretical study. <i>Inorganica Chimica Acta</i> , 2021, 527, 120584. | 1.2 | 2 |
| 15336 | Structural and spectroscopic analysis of the Cis-Trans isomers of the captopril in the gaseous and aqueous phases. <i>Journal of Molecular Structure</i> , 2021, 1243, 130872. | 1.8 | 2 |
| 15337 | Large relativistic effects in ^{119}Sn NMR parameters: A case study of complex anions $[Cp^*M(SnCl_3)_nCl_3]^{n-}$, where $M = Rh, Ir$; $n = 1, 2, 3$. <i>Computational and Theoretical Chemistry</i> , 2021, 1205, 113432. | 1.1 | 4 |
| 15338 | Tuning the structure of pyridinolate-based functional ionic liquids for highly efficient SO_2 absorption. <i>Fuel</i> , 2021, 303, 121311. | 3.4 | 21 |
| 15339 | Selective synthesis of $Ni_{12}P_5$ and Ni_2P nanoparticles: Electronic structures, magnetic and optical properties. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2021, 273, 115389. | 1.7 | 7 |
| 15340 | Theoretical study of thiophene-inserted COF as high performance anode material for Li-ion battery. <i>Chemical Physics Letters</i> , 2021, 783, 139042. | 1.2 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15341 | Stress degradation mechanism of coal macromolecular structure: Insights from molecular dynamics simulation and quantum chemistry calculations. <i>Fuel</i> , 2021, 303, 121258. | 3.4 | 18 |
| 15342 | DFT studies on the mechanisms of enantioselective Ni-catalyzed reductive coupling reactions to form 1,1-diarylalkanes. <i>Journal of Organometallic Chemistry</i> , 2021, 952, 122042. | 0.8 | 4 |
| 15343 | Highly persistent triphenylamine-based catholyte for durable organic redox flow batteries. <i>Energy Storage Materials</i> , 2021, 42, 185-192. | 9.5 | 13 |
| 15344 | Synthesis, bioinformatics and biological evaluation of novel pyridine based on 8-hydroxyquinoline derivatives as antibacterial agents: DFT, molecular docking and ADME/T studies. <i>Journal of Molecular Structure</i> , 2021, 1244, 130934. | 1.8 | 25 |
| 15345 | Excited state intramolecular proton transfer mechanism of a benzothiazole derivative fluorescent probe: Spontaneous ES IPT process. <i>Chemical Physics Letters</i> , 2021, 783, 139055. | 1.2 | 5 |
| 15346 | Facile and label-free fluorescence strategy for evaluating the influence of bioactive ingredients on FMO3 activity via supramolecular host-guest reporter pair. <i>Biosensors and Bioelectronics</i> , 2021, 192, 113488. | 5.3 | 14 |
| 15347 | An ultrahigh-energy-density lithium metal capacitor. <i>Energy Storage Materials</i> , 2021, 42, 154-163. | 9.5 | 13 |
| 15348 | Predicting ion mobility as a function of the electric field for small ions in light gases. <i>Analytica Chimica Acta</i> , 2021, 1184, 339019. | 2.6 | 9 |
| 15349 | Unravelling the diarsenic hydrides: Reactivity and spectroscopic properties. <i>Journal of Molecular Structure</i> , 2021, 1244, 130971. | 1.8 | 2 |
| 15350 | Influence of progressive halogenation of Zn(II)-tetraarylporphyrins and their free bases on the structure and spectral-fluorescence properties of tetrapyrrolic macrocycle. <i>Inorganica Chimica Acta</i> , 2021, 528, 120620. | 1.2 | 1 |
| 15351 | Experimental and computational Raman spectroscopies applied to 2-methoxy-2-methylpropylisocyanide (MIBI) ligand of the ^{99m} Tc-sestamibi radiopharmaceutical. <i>Journal of Molecular Structure</i> , 2021, 1246, 131159. | 1.8 | 2 |
| 15352 | A new Organic-Inorganic hybrid compound (NH ₃ (CH ₂) ₂ C ₆ H ₅) ₂ [SnCl ₆]: Crystal structure, characterization, Hirshfeld surface analysis, DFT calculation, vibrational properties and biological evaluation. <i>Journal of Solid State Chemistry</i> , 2021, 304, 122587. | 1.4 | 6 |
| 15353 | Electronic structure and stability of hexanuclear complex [Cu ₆ (hfa) ₄ (dpm) ₄ (OH) ₄]. <i>Journal of Molecular Structure</i> , 2021, 1245, 131116. | 1.8 | 1 |
| 15354 | Pincer-like pyrazole- and imidazole-pyridinyl compounds: Synthesis, characterisation, crystallographic and computational investigation. <i>Journal of Molecular Structure</i> , 2021, 1245, 131147. | 1.8 | 0 |
| 15355 | Investigation of structural, electronical and in vitro cytotoxic activity properties of some heterocyclic compounds. <i>Journal of Molecular Structure</i> , 2021, 1246, 131127. | 1.8 | 13 |
| 15356 | Ultrahigh rate and high-performance lithium-sulfur batteries with resorcinol-formaldehyde xerogel derived highly porous carbon matrix as sulfur cathode host. <i>Chemical Engineering Journal</i> , 2021, 425, 131521. | 6.6 | 21 |
| 15357 | Experimental and DFT investigation on N-functionalized biochars for enhanced removal of Cr(VI). <i>Environmental Pollution</i> , 2021, 291, 118244. | 3.7 | 15 |
| 15358 | 3-(1,3-Dioxoisindolin-2-yl)-N,N-dimethylpropan-1-ammonium perchlorate: Synthesis, crystal structure, docking study and in vitro anticancer activity against the human hepatomas cell line (Hep G2). <i>Journal of Molecular Structure</i> , 2021, 1245, 131006. | 1.8 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15359 | Rationally constructing of a novel composite photocatalyst with multi charge transfer channels for highly efficient sulfamethoxazole elimination: Mechanism, degradation pathway and DFT calculation. <i>Chemical Engineering Journal</i> , 2021, 426, 131585. | 6.6 | 89 |
| 15360 | N-diethylaminosalicylidene based fluorescent Schiff base chemosensor for Al ³⁺ ion: Synthesis, characterisation and DFT/TD-DFT studies. <i>Journal of Molecular Structure</i> , 2022, 1247, 131257. | 1.8 | 30 |
| 15361 | Quantum chemical prediction of effects of temperature on hydrolysis rate of penicillin under weakly acidic condition. <i>Science of the Total Environment</i> , 2022, 806, 150509. | 3.9 | 1 |
| 15362 | Effect anions on the hydrogenation of nitrobenzene over N-rich Poly(ionic liquid) supported Pd catalyst. <i>Chemical Engineering Journal</i> , 2022, 429, 132224. | 6.6 | 23 |
| 15363 | Aggregation induced by the synergy of sodium chloride and high-pressure improves chlorophyll stability. <i>Food Chemistry</i> , 2022, 366, 130577. | 4.2 | 14 |
| 15364 | Critical influences of metal compounds on the formation and stabilization of environmentally persistent free radicals. <i>Chemical Engineering Journal</i> , 2022, 427, 131666. | 6.6 | 28 |
| 15365 | Pressure dependent phase transformations of energetic material 2,4-dinitroanisole using Raman spectroscopy, X-ray diffraction and first principles calculations. <i>Journal of Molecular Structure</i> , 2022, 1247, 131356. | 1.8 | 3 |
| 15366 | Mechanochemical bromination of unburned carbon in fly ash and its mercury removal mechanism: DFT study. <i>Journal of Hazardous Materials</i> , 2022, 423, 127198. | 6.5 | 19 |
| 15367 | Optical properties of new 5- (phenothiazinyl)methylidenebarbituric acid derivatives. <i>Journal of Molecular Structure</i> , 2022, 1247, 131334. | 1.8 | 1 |
| 15368 | Vibrational spectral analysis of Sorafenib and its molecular docking study compared to other TKIs. <i>Journal of Molecular Structure</i> , 2022, 1248, 131507. | 1.8 | 4 |
| 15369 | Effectively controlling the ESIPT behavior and fluorescence feature of 2-(2-hydroxyphenyl)-4-chloromethylthiazole by changing its π -conjugation: A theoretical exploration. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 422, 113548. | 2.0 | 9 |
| 15370 | Synthesis, physicochemical properties, crystal molecular structure and DFT investigation of an organobismuth(III) bis(dimethyldithiocarbamate) and its organolithium precursor. <i>Journal of Molecular Structure</i> , 2022, 1247, 131335. | 1.8 | 1 |
| 15371 | Novel Compounds Based on Chalcone- and Pyrazoline-DIM Hybrids as Inhibitors of <i>Staphylococcus aureus</i> , Synthesis, DFT Studies, Biological Evaluation and Docking Studies. <i>Journal of Molecular Structure</i> , 2022, 1249, 131499. | 1.8 | 6 |
| 15372 | Synthesis and spectral properties of near-infrared cyanine dyes showing enhanced Stokes shift: A paradigm of ICT dipolar state polymethine chromophoric systems. <i>Journal of Molecular Structure</i> , 2022, 1247, 131381. | 1.8 | 4 |
| 15373 | Structure, morphology and modelling studies of polyvinylalcohol nanocomposites reinforced with nickel oxide nanoparticles and graphene quantum dots. <i>Environmental Research</i> , 2022, 203, 111842. | 3.7 | 28 |
| 15374 | N-Donor stabilized tin(II) cations as efficient ROP catalysts for the synthesis of linear and star-shaped PLAs via the activated monomer mechanism. <i>Dalton Transactions</i> , 2021, 50, 16039-16052. | 1.6 | 5 |
| 15375 | New Hybrid Copper Nanoparticles/Conjugated Polyelectrolyte Composite with Antibacterial Activity. <i>Polymers</i> , 2021, 13, 401. | 2.0 | 7 |
| 15376 | Enantioselective synthesis of chiral tetrasubstituted allenes: harnessing electrostatic and noncovalent interactions in a bifunctional activation model for N-triflylphosphoramidate catalysis. <i>Organic Chemistry Frontiers</i> , 2021, 8, 1510-1519. | 2.3 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15377 | Theoretical analysis of means of preventing Siâ€C bond cleavage during polycondensation of organosilanes to organosilicas. <i>New Journal of Chemistry</i> , 2021, 45, 6120-6128. | 1.4 | 1 |
| 15378 | Ibuprofen-loaded biocompatible latex membrane for drug release: Characterization and molecular modeling. <i>Journal of Applied Biomaterials and Functional Materials</i> , 2021, 19, 228080002110053. | 0.7 | 7 |
| 15379 | Quinol-containing ligands enable high superoxide dismutase activity by modulating coordination number, charge, oxidation states and stability of manganese complexes throughout redox cycling. <i>Chemical Science</i> , 2021, 12, 10483-10500. | 3.7 | 15 |
| 15380 | <i>o</i> -Semiquinone radical anion isolated as an amorphous porous solid. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17408-17419. | 1.3 | 5 |
| 15381 | Simple models for the quick estimation of ground state hydrogen tunneling splittings in alcohols and other compounds. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17591-17605. | 1.3 | 7 |
| 15382 | Submonomer synthesis of peptoids containing <i>trans</i> -inducing <i>N</i> -imino- and <i>N</i> -alkylamino-glycines. <i>Chemical Science</i> , 2021, 12, 8401-8410. | 3.7 | 16 |
| 15383 | The influence mechanism of the molecular structure on the peak current and peak potential in electrochemical detection of typical quinolone antibiotics. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13873-13877. | 1.3 | 7 |
| 15384 | A study of products of tetrakis(hydroxymethyl)glycoluril dehydroxymethylation in aqueous solutions. <i>Russian Chemical Bulletin</i> , 2021, 70, 140-147. | 0.4 | 4 |
| 15385 | Magnetic properties of organolanthanide(ii) complexes, from the electronic structure and the crystal field effect. <i>Dalton Transactions</i> , 2021, 50, 9787-9795. | 1.6 | 0 |
| 15386 | A computational study of the properties of low- and high-index Pd, Cu and Zn surfaces. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 14649-14661. | 1.3 | 5 |
| 15387 | Comment on "Theoretical investigation on bond and spectrum of cyclo[18]carbon (C18) with sp-hybridized". <i>Journal of Molecular Modeling</i> , 2021, 27, 42. | 0.8 | 23 |
| 15388 | Quantifying Uncertainties in Solvation Procedures for Modeling Aqueous Phase Reaction Mechanisms. <i>Journal of Physical Chemistry A</i> , 2021, 125, 154-164. | 1.1 | 24 |
| 15389 | Conformationally rigid molecular and polymeric naphthalene-diimides containing C ₆ H ₆ N ₂ constitutional isomers. <i>Journal of Materials Chemistry C</i> , 2021, 9, 10875-10888. | 2.7 | 7 |
| 15390 | The CH ₂ CH ₂ + OH Gas Phase Reaction: Formaldehyde and Acetaldehyde Formation Routes. <i>Lecture Notes in Computer Science</i> , 2021, , 581-593. | 1.0 | 0 |
| 15391 | Long-Range Complex in the HC ₃ N + CN Potential Energy Surface: Ab Initio Calculations and Intermolecular Potential. <i>Lecture Notes in Computer Science</i> , 2021, , 413-425. | 1.0 | 2 |
| 15392 | Hydride Affinities for Main-Group Hydride Reductants: Assessment of Density Functionals and Trends in Reactivities. <i>Journal of Physical Chemistry A</i> , 2021, 125, 835-842. | 1.1 | 7 |
| 15393 | Efficient evaluation of electrostatic potential with computerized optimized code. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20323-20328. | 1.3 | 664 |
| 15394 | Disentangling the complex network of non-covalent interactions in fenchone hydrates <i>via</i> rotational spectroscopy and quantum chemistry. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20686-20694. | 1.3 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15395 | Dâ€“â€“A type ferrocene-substituted azobenzene photochromic switches: synthesis, structures, and electrochemical and photoisomerization studies. <i>New Journal of Chemistry</i> , 2021, 45, 19917-19927. | 1.4 | 3 |
| 15396 | Benchmarking TD-DFT and Wave Function Methods for Oscillator Strengths and Excited-State Dipole Moments. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1117-1132. | 2.3 | 88 |
| 15397 | Electronic Properties of Doped Graphene Nanoribbon and the Electron Distribution Contours: A DFT Study. <i>Russian Journal of Physical Chemistry B</i> , 2021, 15, 46-52. | 0.2 | 6 |
| 15398 | Study on the Decomposition Pathways and Products of C4F7N/N2. <i>Lecture Notes in Electrical Engineering</i> , 2021, , 157-164. | 0.3 | 0 |
| 15399 | Basis Sets for Heavy Atoms. <i>Lecture Notes in Quantum Chemistry II</i> , 2021, , 183-214. | 0.3 | 7 |
| 15400 | Computational modelling of Pd-catalysed alkoxy carbonylation of alkenes and alkynes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15869-15880. | 1.3 | 7 |
| 15401 | Effect of electron-withdrawing groups on molecular properties of naphthyl and anthryl bithiophenes as potential n-type semiconductors. <i>New Journal of Chemistry</i> , 2021, 45, 9794-9804. | 1.4 | 12 |
| 15402 | From Y6 to BTPT-4F: a theoretical insight into the influence of the individual change of fused-ring skeleton length or side alkyl chains on molecular arrangements and electron mobility. <i>New Journal of Chemistry</i> , 2021, 45, 12247-12259. | 1.4 | 9 |
| 15403 | RNA-targeting low-molecular-weight fluorophores for nucleoli staining: synthesis, <i>in silico</i> modelling and cellular imaging. <i>New Journal of Chemistry</i> , 2021, 45, 12818-12829. | 1.4 | 7 |
| 15404 | Photoreduction Mechanism of CO ₂ to CO Catalyzed by a Three-Component Hybrid Construct with a Bimetallic Rhenium Catalyst. <i>ACS Catalysis</i> , 2021, 11, 1495-1504. | 5.5 | 19 |
| 15405 | Synthesis, characterization and ab initio study of WO ₃ nanocubes with peculiar electrochemical properties. <i>Journal of Nanoparticle Research</i> , 2021, 23, 1. | 0.8 | 6 |
| 15406 | Disclosing the hierarchical structure of ionic liquid mixtures by multiscale computational methods. , 2021, , 1-67. | | 1 |
| 15407 | Amphipathic 1,3-oxazolidines from N-alkyl glucamines and benzaldehydes: stereochemical and mechanistic studies. <i>New Journal of Chemistry</i> , 2021, 45, 4365-4386. | 1.4 | 2 |
| 15408 | Experimental and theoretical studies of 1,3,5-tris (bromomethyl)-2,4,6-trimethylbenzene with 2-â€“pyridone. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4188. | 0.9 | 1 |
| 15409 | Surface modification of polyamide reverse osmosis membranes with small-molecule zwitterions for enhanced fouling resistance: a molecular simulation study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6623-6631. | 1.3 | 7 |
| 15410 | Design of a fluorescent and clickable Ag ₃₈ (SRN ₃) ₂₄ nanocluster platform: synthesis, modeling and self-assembling. <i>Nanoscale Advances</i> , 2021, 3, 2948-2960. | 2.2 | 2 |
| 15411 | Computational study on the mechanism of hydroboration of CO ₂ catalysed by POCOP pincer nickel thiolate complexes: concerted catalysis and hydride transfer by a shuttle. <i>Dalton Transactions</i> , 2021, 50, 2903-2914. | 1.6 | 11 |
| 15412 | Understanding Structural and Transport Properties of Dissolved Li ₂ S ₈ in Ionic Liquid Electrolytes through Molecular Dynamics Simulations. <i>ChemPhysChem</i> , 2021, 22, 419-429. | 1.0 | 16 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15413 | Machine learning to tame divergent density functional approximations: a new path to consensus materials design principles. <i>Chemical Science</i> , 2021, 12, 13021-13036. | 3.7 | 23 |
| 15414 | Structure optimization of lipopeptide assemblies for aldol reactions in an aqueous medium. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10953-10963. | 1.3 | 2 |
| 15415 | Protective interlayer for trapping polysulfides and a conducting host for sulfur: dual role of candle soot carbon for the development of high performance lithium-sulfur batteries. <i>Materials Advances</i> , 2021, 2, 3031-3041. | 2.6 | 12 |
| 15416 | Kinetic modeling of nitrous oxide decomposition on Fe-ZSM-5 in the presence of nitric oxide based on parameters obtained from first-principles calculations. <i>Catalysis Science and Technology</i> , 2021, 11, 3539-3555. | 2.1 | 3 |
| 15417 | Aromaticity in molecules and transition structures: from atomic and molecular orbitals to simple ring current models. , 2021, , 1-41. | | 0 |
| 15418 | High-throughput virtual screening for organic electronics: a comparative study of alternative strategies. <i>Journal of Materials Chemistry C</i> , 2021, 9, 13557-13583. | 2.7 | 20 |
| 15419 | Distiboranes based on <i>ortho</i> -phenylene backbones as bidentate Lewis acids for fluoride anion chelation. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 4949-4957. | 1.5 | 14 |
| 15420 | DFT Mechanism of Cu Catalyzed Coupling Reaction to Alkyl Aryl Ethers. <i>Acta Chimica Sinica</i> , 2021, 79, 948. | 0.5 | 1 |
| 15421 | Unprecedented copper(ii) coordination induced nucleophilic cleavage of a quinoxaline heterocycle: structural and computational studies. <i>CrystEngComm</i> , 2021, 23, 5078-5086. | 1.3 | 3 |
| 15422 | Pros and cons of the time-dependent hybrid density functional approach for calculating the optical spectra of solids: a case study of CeO ₂ . <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16296-16306. | 1.3 | 5 |
| 15423 | Polycyclic aromatic hydrocarbons: from small molecules through nano-sized species towards bulk graphene. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17713-17723. | 1.3 | 13 |
| 15424 | Predicting ligand removal energetics in thiolate-protected nanoclusters from molecular complexes. <i>Nanoscale</i> , 2021, 13, 2034-2043. | 2.8 | 7 |
| 15425 | Determining electron-nucleus distances and Fermi contact couplings from ENDOR spectra. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8326-8335. | 1.3 | 5 |
| 15426 | Ground and excited electronic structures of metal encapsulated nanocages: the cases of endohedral M@C ₂₀ H ₂₀ (M = K, Rb, Ca, Sr) and M@C ₃₆ H ₃₆ (M = Na, Tl). <i>Chemical Physics Letters</i> , 2021, 743, 107843. | 1.0 | 1 |
| 15427 | Hydroxido supported and differently networked octanuclear Ni ₆ Ln ₂ [Ln = Gd ^{III} and Dy ^{III}] complexes: structural variation, magnetic properties and theoretical insights. <i>Dalton Transactions</i> , 2021, 50, 5023-5035. | 1.6 | 6 |
| 15428 | How Beneficial Is the <i>Explicit</i> Account of Doubly-Excited Configurations in Linear Response Theory?. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 975-984. | 2.3 | 12 |
| 15429 | Theoretical evaluation of the corrosion inhibition performance of aliphatic dipeptides. <i>New Journal of Chemistry</i> , 2021, 45, 3610-3629. | 1.4 | 11 |
| 15430 | Photocatalytic polymers of intrinsic microporosity for hydrogen production from water. <i>Journal of Materials Chemistry A</i> , 2021, 9, 19958-19964. | 5.2 | 36 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15431 | Quantitative insights into the phase behaviour and miscibility of organic photovoltaic active layers from the perspective of neutron spectroscopy. <i>Journal of Materials Chemistry C</i> , 2021, 9, 11873-11881. | 2.7 | 2 |
| 15432 | Predicting OH stretching fundamental wavenumbers of alcohols for conformational assignment: different correction patterns for density functional and wave-function-based methods. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5629-5643. | 1.3 | 11 |
| 15433 | Modelling biocompatible ionic liquids based on organic acids and amino acids: challenges for computational models and future perspectives. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 4002-4013. | 1.5 | 7 |
| 15434 | Can the sensitivity of energetic materials be tuned by using hydrogen bonds? Another look at the role of hydrogen bonding in the design of high energetic compounds. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7472-7479. | 1.3 | 16 |
| 15435 | An insight into the reaction mechanism of CO ₂ photoreduction catalyzed by atomically dispersed Fe atoms supported on graphitic carbon nitride. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4690-4699. | 1.3 | 22 |
| 15437 | From Cyclopentasilane to Thin-Film Transistors. <i>Advanced Electronic Materials</i> , 2021, 7, 2000422. | 2.6 | 4 |
| 15438 | Oxidation, Coordination, and Nickel-Mediated Deconstruction of a Highly Electron-Rich Diboron Analogue of 1,3,5-Hexatriene. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15717-15725. | 7.2 | 14 |
| 15439 | Spin-State Energetics of Fe Complexes from an Optimally Tuned Range-Separated Hybrid Functional. <i>Chemistry - A European Journal</i> , 2018, 24, 5173-5182. | 1.7 | 38 |
| 15440 | Halogenated Alkyltetrazoles for the Rational Design of Fe ^{II} Spin-Crossover Materials: Fine-Tuning of the Ligand Size. <i>Chemistry - A European Journal</i> , 2018, 24, 5271-5280. | 1.7 | 8 |
| 15441 | Mono- and Bivalent 14- β Inhibitors for Characterizing Supramolecular α -Lysine Wrapping of Oligoethylene Glycol (OEG) Moieties in Proteins. <i>Chemistry - A European Journal</i> , 2018, 24, 13807-13814. | 1.7 | 6 |
| 15442 | Local Aromaticity in Polycyclic Aromatic Hydrocarbons: Electron Delocalization versus Magnetic Indices. <i>Chemistry - A European Journal</i> , 2006, , . | 1.7 | 1 |
| 15443 | Reactivity of Copper(III)-Oxo Complexes in the Gas Phase. <i>ChemPhysChem</i> , 2017, 18, 2217-2224. | 1.0 | 17 |
| 15444 | Theoretical study of intramolecular hydrogen bonding and molecular geometry of 2-trifluoromethylphenol. <i>Journal of Computational Chemistry</i> , 1996, 17, 1804-1819. | 1.5 | 15 |
| 15445 | Synthesis, Structure, and DFT Analysis of the THF Solvate of 2-Picolylithium: A 2-Picolylithium Solvate with Significant Carbanionic Character. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2020, 646, 726-733. | 0.6 | 5 |
| 15446 | Real Space Ab Initio Calculations of Excitation Energies in Small Silicon Quantum Dots. , 2005, , 317-332. | | 2 |
| 15447 | Hohenberg-Kohn-Sham Density Functional Theory. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2007, , 153-201. | 0.6 | 1 |
| 15448 | Substrate-Enzyme Interactions from Modeling and Isotope Effects. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2007, , 341-363. | 0.6 | 2 |
| 15449 | Theoretical Models of Active Sites: General Considerations and Application to the Study of Phillips-Type Cr/Silica Catalysts for Ethylene Polymerization. <i>Nanostructure Science and Technology</i> , 2005, , 85-111. | 0.1 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15450 | Density-Functional Theory in External Electric and Magnetic Fields. Modern Aspects of Electrochemistry, 2009, , 341-408. | 0.2 | 1 |
| 15451 | Density Functional and Neural Network Analysis. , 1997, , 255-277. | | 13 |
| 15452 | Quantum Mechanical Methods for the Investigation of Metalloproteins and Related Bioinorganic Compounds. Methods in Molecular Biology, 2014, 1122, 207-268. | 0.4 | 2 |
| 15453 | A Computational Study of the Reaction Cyanoacetylene and Cyano Radical Leading to 2-Butynedinitrile and Hydrogen Radical. Lecture Notes in Computer Science, 2020, , 707-716. | 1.0 | 3 |
| 15454 | A Theoretical Investigation of the Reactions of N(2D) with Small Alkynes and Implications for the Prebiotic Chemistry of Titan. Lecture Notes in Computer Science, 2020, , 717-729. | 1.0 | 3 |
| 15455 | A Computational Study on the Insertion of N(2D) into a C-H or C-C Bond: The Reactions of N(2D) with Benzene and Toluene and Their Implications on the Chemistry of Titan. Lecture Notes in Computer Science, 2020, , 744-755. | 1.0 | 7 |
| 15456 | Innovations in Finite-Temperature Density Functionals. Lecture Notes in Computational Science and Engineering, 2014, , 61-85. | 0.1 | 4 |
| 15457 | Density Functional Calculations. , 2016, , 483-563. | | 1 |
| 15458 | Review on Simulation Models for Materials and Biomolecular Study and Design. , 2017, , 373-408. | | 3 |
| 15459 | Computational Studies on Osmium-Catalyzed Olefin Oxidation Reactions. , 2012, , 143-168. | | 1 |
| 15460 | Exact decoupling of the relativistic Fock operator. , 2012, , 205-224. | | 2 |
| 15461 | Theoretical and Experimental Study of the Energy and Structure of Fragment Ions Produced by Double Photoionization of Benzene Molecules. Lecture Notes in Computer Science, 2012, , 316-330. | 1.0 | 3 |
| 15462 | Theoretical Study of Reactions Relevant for Atmospheric Models of Titan: Interaction of Excited Nitrogen Atoms with Small Hydrocarbons. Lecture Notes in Computer Science, 2012, , 331-344. | 1.0 | 19 |
| 15463 | Towards Model-Based Design of Tailor-Made Fuels from Biomass. Notes on Numerical Fluid Mechanics and Multidisciplinary Design, 2015, , 193-211. | 0.2 | 3 |
| 15464 | On the Performance of a Size-Extensive Variant of Equation-of-Motion Coupled Cluster Theory for Optical Rotation in Chiral Molecules. Progress in Theoretical Chemistry and Physics, 2009, , 225-239. | 0.2 | 9 |
| 15465 | Divide-and-Conquer Approaches to Quantum Chemistry: Theory and Implementation. Challenges and Advances in Computational Chemistry and Physics, 2011, , 97-127. | 0.6 | 27 |
| 15466 | Computational Perspectives on Organolithium Carbenoids. , 2012, , 471-510. | | 4 |
| 15467 | First Steps Towards Quantum Refinement of Protein X-Ray Structures. , 2012, , 87-120. | | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15468 | Description of Core-Ionized and Core-Excited States by Density Functional Theory and Time-Dependent Density Functional Theory. <i>Progress in Theoretical Chemistry and Physics</i> , 2012, , 275-308. | 0.2 | 2 |
| 15469 | Auxiliary Density Functional Theory: From Molecules to Nanostructures. , 2015, , 1-67. | | 5 |
| 15470 | Quantum Chemical Studies of Transition Metal Catalyzed Enzyme Reactions. , 1997, , 233-253. | | 4 |
| 15471 | Vibrational Circular Dichroism of Nucleic Acids. , 1997, , 299-317. | | 2 |
| 15472 | Accurate Calculation of the Interaction Energies in Hydrogen-Bonded Complexes. , 2000, , 35-44. | | 7 |
| 15473 | Tautomeric and epimeric equilibria of aldo- and ketohexoses studied by the MD simulations and QM calculations. <i>Carbohydrate Research</i> , 2019, 474, 8-15. | 1.1 | 4 |
| 15474 | Molecular simulation of the separation of toluene and p-xylene with the thermally-robust ionic liquid triphenyl-p-phenyl sulfonyl phenyl phosphonium. <i>Chemical Engineering Science</i> , 2020, 224, 115790. | 1.9 | 8 |
| 15475 | Photocontrol of Endogenous Glycine Receptors In Vivo. <i>Cell Chemical Biology</i> , 2020, 27, 1425-1433.e7. | 2.5 | 16 |
| 15476 | Use of dual-filtering to create training sets leading to improved accuracy in quantitative structure-retention relationships modelling for hydrophilic interaction liquid chromatographic systems. <i>Journal of Chromatography A</i> , 2017, 1507, 53-62. | 1.8 | 26 |
| 15477 | Reactions of cisplatin and cis-[PtI ₂ (NH ₃) ₂] with molecular models of relevant protein sidechains: A comparative analysis. <i>Journal of Inorganic Biochemistry</i> , 2020, 209, 111096. | 1.5 | 22 |
| 15479 | Straight Z and twisted E isomers from triphenylamine derivatives: Intramolecular charge transfer and second-order nonlinear optical response. <i>Journal of Molecular Liquids</i> , 2020, 311, 113297. | 2.3 | 9 |
| 15480 | Evaluation of the substitution structures of two partially fluorinated cyclopentanes C ₅ H ₃ F ₇ and C ₅ H ₂ F ₈ . <i>Journal of Molecular Structure</i> , 2020, 1207, 127778. | 1.8 | 2 |
| 15481 | Synthesis, crystal structure, antibacterial, antiproliferative and QSAR studies of new bismuth(III) complexes of pyrrolidinedithiocarbamate of dithia-bismolane and bismane, oxodithia- and trithia-bismocane. <i>Journal of Molecular Structure</i> , 2020, 1217, 128456. | 1.8 | 9 |
| 15482 | Vibrational Spectroscopic Studies of Nitrated Polycyclic Aromatic Hydrocarbons (NPAHs): A Review (1960-2019). <i>Vibrational Spectroscopy</i> , 2020, 109, 103072. | 1.2 | 4 |
| 15483 | Degradation of Pharmaceuticals through Sequential Photon Absorption and Photoionization in Amiloride Derivatives. <i>Cell Reports Physical Science</i> , 2020, 1, 100274. | 2.8 | 5 |
| 15484 | Stability constants of Sb ⁵⁺ with Cl ⁻ and thermodynamics of Sb ⁵⁺ -Cl ⁻ -H ₂ O system involving complex behavior of Sb with Cl. <i>Transactions of Nonferrous Metals Society of China</i> , 2020, 30, 3379-3389. | 1.7 | 5 |
| 15485 | Tuning Ionic Liquids with Functional Anions for SO ₂ Capture through Simultaneous Cooperation of N and O Chemical Active Sites with SO ₂ . <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 21522-21529. | 1.8 | 21 |
| 15486 | Insight into the Substitution Mechanism of Antitumor Au(I) N-Heterocyclic Carbene Complexes by Cysteine and Selenocysteine. <i>Inorganic Chemistry</i> , 2020, 59, 3312-3320. | 1.9 | 27 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15487 | Toward a Neutral Single-Component Amidinate Iodide Aluminum Catalyst for the CO ₂ Fixation into Cyclic Carbonates. <i>Inorganic Chemistry</i> , 2021, 60, 1172-1182. | 1.9 | 18 |
| 15488 | Thermochemical Data Fusion Using Graph Representation Learning. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4673-4683. | 2.5 | 5 |
| 15489 | Energy Landscapes for Electronic Structure. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 151-169. | 2.3 | 18 |
| 15490 | Generalization of Block-Localized Wave Function for Constrained Optimization of Excited Determinants. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 277-289. | 2.3 | 18 |
| 15491 | A Route to Triazole-Fused Sultams via Metal-Free Base-Mediated Cyclization of Sulfonamide-Tethered 5-Iodotriazoles. <i>Journal of Organic Chemistry</i> , 2020, 85, 7863-7876. | 1.7 | 17 |
| 15493 | Solid-State ¹⁷ O NMR Studies of Sulfonate Jump Dynamics in Crystalline Sulfonic Acids: Insights into the Hydrogen Bonding Effect. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9597-9604. | 1.1 | 7 |
| 15494 | Structural Evolution and Electronic Properties of TaSi ₁₀ ($\epsilon = 1$). <i>Journal of Physical Chemistry A</i> , 2020, 124, 9818-9831. | 1.1 | 18 |
| 15495 | Fluorescence Anisotropy Detection of Barrier Crossing and Ultrafast Conformational Dynamics in the S ₂ State of ¹² -Carotene. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9029-9046. | 1.2 | 10 |
| 15496 | TICT-Based Near-Infrared Ratiometric Organic Fluorescent Thermometer for Intracellular Temperature Sensing. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 26842-26851. | 4.0 | 70 |
| 15497 | Unimolecular Fragmentation Properties of Thermometer Ions from Chemical Dynamics Simulations. <i>Journal of the American Society for Mass Spectrometry</i> , 2021, 32, 169-179. | 1.2 | 5 |
| 15498 | CHAPTER 12. Real-time and Real-space Time-dependent Density-functional Theory Approach to Attosecond Dynamics. <i>RSC Theoretical and Computational Chemistry Series</i> , 0, , 424-461. | 0.7 | 3 |
| 15499 | Theoretical and physical aspects of nuclear shielding. <i>Nuclear Magnetic Resonance</i> , 2012, , 38-55. | 0.1 | 3 |
| 15500 | Synthesis of 3,3-disubstituted oxindoles by one-pot integrated Brønsted base-catalyzed trichloroacetimidation of 3-hydroxyoxindoles and Brønsted acid-catalyzed nucleophilic substitution reaction. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 1533. | 1.5 | 41 |
| 15501 | BAR-based optimum adaptive sampling regime for variance minimization in alchemical transformation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15005-15020. | 1.3 | 41 |
| 15502 | Heavy ligand atom induced large magnetic anisotropy in Mn(σ) complexes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 16914-16922. | 1.3 | 12 |
| 15503 | Polyaniline and CN-functionalized polyaniline as organic cathodes for lithium and sodium ion batteries: a combined molecular dynamics and density functional tight binding study in solid state. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 232-237. | 1.3 | 27 |
| 15504 | Synthesis and redox reactions of bis(verdazyl)palladium complexes. <i>Dalton Transactions</i> , 2017, 46, 12636-12644. | 1.6 | 15 |
| 15505 | Comparing the performances of various density functionals for modelling the mechanisms and kinetics of bimolecular free radical reactions in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23425-23440. | 1.3 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15506 | A highly sensitive and selective colorimetric probe based on a cycloruthenated complex: an Hg ²⁺ -promoted switch of thiophene coordination. Dalton Transactions, 2020, 49, 2024-2032. | 1.6 | 4 |
| 15507 | Experimental and DFT studies on the ultrasonic energy-assisted extraction of the phytochemicals of <i>Catharanthus roseus</i> as green corrosion inhibitors for mild steel in NaCl medium. RSC Advances, 2020, 10, 5399-5411. | 1.7 | 31 |
| 15508 | Boron-containing D ⁴ A type TADF materials with tiny singlet-triplet energy splittings and high photoluminescence quantum yields for highly efficient OLEDs with low efficiency roll-offs. Journal of Materials Chemistry C, 2020, 8, 3846-3854. | 2.7 | 26 |
| 15509 | Electronic and spin structures of CaMn ₄ O _x clusters in the S ₀ state of the oxygen evolving complex of photosystem II. Domain-based local pair natural orbital (DLPNO) coupled-cluster (CC) calculations using optimized geometries and natural orbitals (UNO) by hybrid density functional theory (HDFT) calculations. Physical Chemistry Chemical Physics, 2020, 22, 27191-27205. | 1.3 | 5 |
| 15510 | Understanding benzyl alcohol aggregation by chiral modification: the pairing step. Physical Chemistry Chemical Physics, 2020, 22, 25538-25551. | 1.3 | 15 |
| 15511 | Quantifying soft degrees of freedom in volatile organic compounds: insight from quantum chemistry and focused single molecule experiments. Physical Chemistry Chemical Physics, 2020, 22, 27850-27860. | 1.3 | 2 |
| 15512 | DOPC versus DOPE as a helper lipid for gene-therapies: molecular dynamics simulations with DLin-MC3-DMA. Physical Chemistry Chemical Physics, 2020, 22, 28256-28268. | 1.3 | 37 |
| 15513 | Understanding the structures and aromaticity of heteroporphyrins with computations. Organic and Biomolecular Chemistry, 2020, 18, 4415-4422. | 1.5 | 7 |
| 15514 | The ortho-to-para ratio of H ₂ Cl ⁺ : Quasi-classical trajectory calculations and new simulations in light of new observations. Astronomy and Astrophysics, 2017, 608, A96. | 2.1 | 6 |
| 15515 | Relative thermodynamic stability of the [C,N,O] linkages as an indication of the most abundant structures in the ISM. Astronomy and Astrophysics, 2020, 639, A16. | 2.1 | 8 |
| 15516 | Testing the α -PAHs hypothesis. Astronomy and Astrophysics, 2003, 410, 639-648. | 2.1 | 22 |
| 15517 | Real-space visualization of conformation-independent oligothiophene electronic structure. Journal of Chemical Physics, 2016, 144, 194703. | 1.2 | 5 |
| 15518 | Screening methods for linear-scaling short-range hybrid calculations on CPU and GPU architectures. Journal of Chemical Physics, 2017, 146, 144108. | 1.2 | 6 |
| 15519 | Temperature dependence of band gaps and conformational disorder in PEDOT and its selenium and tellurium derivatives: Density functional calculations. Journal of Chemical Physics, 2017, 147, 134906. | 1.2 | 6 |
| 15520 | Screened range-separated hybrid by balancing the compact and slowly varying density regimes: Satisfaction of local density linear response. Journal of Chemical Physics, 2020, 152, 044111. | 1.2 | 22 |
| 15521 | Separation of electron-electron and electron-proton correlation in multicomponent orbital-optimized perturbation theory. Journal of Chemical Physics, 2020, 152, 194107. | 1.2 | 12 |
| 15522 | Toward a systematic improvement of the fixed-node approximation in diffusion Monte Carlo for solids: A case study in diamond. Journal of Chemical Physics, 2020, 153, 184111. | 1.2 | 16 |
| 15523 | Unveiling the coexistence of <i>cis</i> - and <i>trans</i> -isomers in the hydrolysis of ZrO ₂ : A coupled DFT and high-resolution photoelectron spectroscopy study. Journal of Chemical Physics, 2020, 153, 244308. | 1.2 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15524 | A Sesquiterpene Isonitrile with a New Tricyclic Skeleton from the Indo-Pacific Nudibranch <i>Phyllidiella pustulosa</i> : Spectroscopic and Computational Studies. <i>Australian Journal of Chemistry</i> , 2020, 73, 129. | 0.5 | 9 |
| 15525 | Synthesis, quantum chemical calculations and molecular docking studies of 2-ethoxy-4[(2-trifluoromethyl-phenylimino)methyl]phenol. <i>Molecular Physics</i> , 2020, 118, . | 0.8 | 10 |
| 15526 | Ab initio calculation of atomic axial tensors and vibrational rotational strengths using density functional theory. <i>Molecular Physics</i> , 1996, 89, 579-594. | 0.8 | 31 |
| 15527 | Ab initio molecular dynamics simulation of H ₅ O ⁺ 2 and H ₇ O ⁺ 3 gas phase clusters based on density functional theory. <i>Molecular Physics</i> , 1997, 91, 963-975. | 0.8 | 29 |
| 15528 | Azoxy rearrangement reactions. <i>Molecular Physics</i> , 1997, 91, 789-804. | 0.8 | 5 |
| 15529 | Potential energy function and vibrational states of HN ₃ and DN ₃ . <i>Molecular Physics</i> , 1998, 93, 853-865. | 0.8 | 19 |
| 15530 | Comparative <i>in vitro</i> and DFT antioxidant studies of phenolic group substituted pyridine-based azo derivatives. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 4921-4932. | 2.0 | 9 |
| 15531 | Modulation of Jahn–Teller distortion and electromechanical response in a Mn ³⁺ spin crossover complex. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 404002. | 0.7 | 13 |
| 15532 | Understanding dynamic properties of materials using neutron spectroscopy and atomistic simulation. <i>Journal of Physics Communications</i> , 2020, 4, 072001. | 0.5 | 21 |
| 15533 | Thousands of reactants and transition states for competing E2 and S _N 2 reactions. <i>Machine Learning: Science and Technology</i> , 2020, 1, 045026. | 2.4 | 33 |
| 15535 | Routes for increasing endurance and retention in HfO_2 -based resistive switching memories. <i>Physical Review Materials</i> , 2018, 2, . | 0.9 | 15 |
| 15536 | Dielectric-dependent hybrid functionals for heterogeneous materials. <i>Physical Review Materials</i> , 2019, 3, . | 0.9 | 36 |
| 15537 | Nanostructure of organic semiconductor thin films: Molecular dynamics modeling with solvent evaporation. <i>Physical Review Materials</i> , 2020, 4, . | 0.9 | 10 |
| 15538 | Optical properties of CsCu | | |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15543 | The many flavours of halogen bonds – message from experimental electron density and Raman spectroscopy. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 1190-1201. | 0.2 | 14 |
| 15544 | Polymer effects on PAG acid yield in EUV resists (Conference Presentation). , 2018, , . | | 4 |
| 15545 | One-Electron Transfer in Reactions of Stable Organic Radicals with Oxygen. <i>Russian Journal of Organic Chemistry</i> , 2020, 56, 2049-2056. | 0.3 | 1 |
| 15546 | Franck-Condon Dominated Chemistry. Formation and Dissociations of the Dimethylhydroxysulfuranyl Radical. <i>Collection of Czechoslovak Chemical Communications</i> , 2000, 65, 455-476. | 1.0 | 21 |
| 15547 | Are There Two Different Geometric Isomers of the O=C=N=C=O Cation?. <i>Collection of Czechoslovak Chemical Communications</i> , 2001, 66, 1038-1046. | 1.0 | 2 |
| 15548 | The Character of Low-Lying Excited States of Mixed-Ligand Metal Carbonyls. TD-DFT and CASSCF/CASPT2 Study of [W(CO)4L] (L = ethylenediamine, N,N'-dialkyl-1,4-diazabutadiene) and [W(CO)5L] (L = pyridine,) Tj ETQq11.1b0.784314 rgBT | | |
| 15549 | Electronic States of Fe2S-/0/+. <i>Collection of Czechoslovak Chemical Communications</i> , 2003, 68, 405-422. | 1.0 | 4 |
| 15550 | 2-Deoxyribose Radicals in the Gas Phase and Aqueous Solution. Transient Intermediates of Hydrogen Atom Abstraction from 2-Deoxyribofuranose. <i>Collection of Czechoslovak Chemical Communications</i> , 2005, 70, 1769-1786. | 1.0 | 5 |
| 15551 | The Mechanism of the Permanganate-Promoted Oxidative Cyclization of 1,5-Dienes - a DFT Study. <i>Collection of Czechoslovak Chemical Communications</i> , 2007, 72, 715-727. | 1.0 | 13 |
| 15552 | A Method for Dimensionally Adaptive Sparse Trigonometric Interpolation of Periodic Functions. <i>SIAM Journal of Scientific Computing</i> , 2020, 42, A2436-A2460. | 1.3 | 8 |
| 15553 | Vibrational Circular Dichroism Spectroscopy. , 2003, , . | | 2 |
| 15554 | Vibrational Circular Dichroism of Biopolymers. , 2005, , 253-324. | | 4 |
| 15555 | Structural and Physical Properties of GexAsySe1-x-y Glasses. , 2014, , 109-154. | | 2 |
| 15556 | Cosmic and Atmospheric Nanosilicates. <i>Series in Materials Science and Engineering</i> , 2016, , 369-412. | 0.1 | 1 |
| 15557 | Generalized Charge Decomposition Analysis (GCDA) Method. <i>Journal of Advances in Physical Chemistry</i> , 2015, 04, 111-124. | 0.1 | 134 |
| 15558 | Benchmark assessment of molecular geometries and energies from small molecule force fields. <i>F1000Research</i> , 2020, 9, 1390. | 0.8 | 30 |
| 15559 | Studies of Optical Properties of Protonated Polyazomethine Thin Films. <i>Acta Physica Polonica A</i> , 2011, 120, 939-941. | 0.2 | 1 |
| 15560 | Reference-free polarization-sensitive quantitative phase imaging using single-point optical phase conjugation. <i>Optics Express</i> , 2018, 26, 26858. | 1.7 | 27 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15561 | Quantitative comparison between sub-millisecond time resolution single-molecule FRET measurements and 10-second molecular simulations of a biosensor protein. <i>PLoS Computational Biology</i> , 2020, 16, e1008293. | 1.5 | 14 |
| 15562 | Biapenem Inactivation by B2 Metallo β -Lactamases: Energy Landscape of the Post-Hydrolysis Reactions. <i>PLoS ONE</i> , 2012, 7, e30079. | 1.1 | 14 |
| 15563 | The Outcome of the Oxidations of Unusual Enediamide Motifs Is Governed by the Stabilities of the Intermediate Iminium Ions. <i>PLoS ONE</i> , 2012, 7, e47224. | 1.1 | 3 |
| 15564 | Biapenem Inactivation by B2 Metallo β -Lactamases: Energy Landscape of the Hydrolysis Reaction. <i>PLoS ONE</i> , 2013, 8, e55136. | 1.1 | 11 |
| 15565 | Synthesis, Spectral Characterization and Crystals Structure of some Arsane Derivatives of Gold (I) Complexes: A Comparative Density Functional Theory Study. <i>PLoS ONE</i> , 2015, 10, e0119620. | 1.1 | 4 |
| 15566 | Barrier to internal rotation, symmetry and carbonyl reactivity in methyl 3,3,3-trifluoropyruvate. <i>Zeitschrift Fur Physikalische Chemie</i> , 2020, 234, 1383-1393. | 1.4 | 3 |
| 15567 | Diazo-pyrazole analogues as photosensitizers in dye sensitised solar cells: tuning for a better photovoltaic efficiency using a new modelling strategy using experimental and computational data. <i>Zeitschrift Fur Physikalische Chemie</i> , 2021, 235, 1227-1245. | 1.4 | 11 |
| 15569 | Phosphorylated thiacalixarenes as molecular receptors for QCM sensors of volatile compounds. <i>Functional Materials</i> , 2017, 24, 599-606. | 0.4 | 2 |
| 15570 | Lipophilic and physicochemical properties of metalloporphyrins separated by RP-TLC. <i>Journal of Planar Chromatography - Modern TLC</i> , 2007, 20, 361-364. | 0.6 | 3 |
| 15571 | Topological Analysis and Frequency Dependent Hyperpolarizability Calculations of FDDNP: a DFT Study. <i>Chemistry Journal of Moldova</i> , 2016, 11, 84-92. | 0.3 | 1 |
| 15572 | DFT Study of the Mechanisms of Transition-Metal-Catalyzed Reductive Coupling Reactions. <i>Current Organic Chemistry</i> , 2020, 24, 1367-1383. | 0.9 | 5 |
| 15573 | Theoretical Study of the Linear Short-Chain Phosphazene-Na ⁺ Complexes. <i>The Open Structural Biology Journal</i> , 2009, 3, 26-33. | 0.1 | 3 |
| 15574 | Theoretical Investigation of the Structural Properties of Two Crodamines Isolated from the Venom of <i>Crotalus durissus</i> . <i>Open Natural Products Journal</i> , 2010, 4, 16-20. | 0.8 | 1 |
| 15575 | Computational Study of Geometry, Solvation Free Energy, Dipole Moment, Polarizability, Hyperpolarizability and Molecular Properties of 2-Methylimidazole. <i>MaÇSallatî ÇŞAmîËzatî Al-Sulá¹Än QÄbÅ«s Li-l-buá, ¥Á«á¹5 Al-Ëjilmıyyatî Al-ËjulÅ«m Wa-al-handasatî</i> , 2017, 21, 89. | | |
| 15576 | A Quantum Chemical Study on Hydration of Ra (II): Comparison with the Other Hydrated Divalent Alkaline Earth Metal Ions. <i>Journal of Computer Chemistry Japan</i> , 2014, 13, 105-113. | 0.0 | 9 |
| 15577 | Absorption of DCM Dye in Ethanol: Experimental and Time Dependent Density Functional Study. <i>International Journal of Optics and Photonics</i> , 2018, 12, 43-56. | 0.2 | 2 |
| 15578 | Gas-Phase TiO ₂ Photosensitized Mineralization of Some VOCs: Mechanistic Suggestions through a Langmuir-Hinshelwood Kinetic Approach. <i>Catalysts</i> , 2021, 11, 20. | 1.6 | 6 |
| 15579 | Kinetic Stability of SiC ₅ H ₂ Isomer with a Planar Tetracoordinate Carbon Atom. <i>Chemistry</i> , 2021, 3, 13-27. | 0.9 | 15 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15580 | How do the Hückel and Baird Rules Fade away in Annulenes?. <i>Molecules</i> , 2020, 25, 711. | 1.7 | 43 |
| 15581 | DNA-Binding Capabilities and Anticancer Activities of Ruthenium(II) Cymene Complexes with (Poly)cyclic Aromatic Diamine Ligands. <i>Molecules</i> , 2021, 26, 76. | 1.7 | 9 |
| 15582 | A Chirality Chain in Phenylglycine, Phenylpropionic Acid, and Ibuprofen. <i>Symmetry</i> , 2021, 13, 55. | 1.1 | 2 |
| 15583 | The Formation of Glycolonitrile (HOCH ₂ CN) from Reactions of C ⁺ with HCN and HNC on Icy Grain Mantles. <i>Astrophysical Journal</i> , 2021, 906, 20. | 1.6 | 9 |
| 15584 | Nucleophilic Substitution Reaction of 5-t-Butyl-2-methoxy-3H-azepine with Alkoxides and Alkylolithium Reagents: A Formation of Bis(5-t-butyl-3H-azepin-2-yl)methane Having a Vinamidine Conjugation. <i>Heterocycles</i> , 2002, 57, 223. | 0.4 | 4 |
| 15585 | Synthesis and Structural Study of Semicarbazone-Containing 1,4-Dihydropyridine. <i>Heterocycles</i> , 2006, 68, 1631. | 0.4 | 4 |
| 15586 | Short Synthesis of (+)-Cylindricine C and Formal Total Synthesis of (-)-Lepadiformine. <i>Heterocycles</i> , 2007, 72, 421. | 0.4 | 29 |
| 15587 | Theoretical Study of Dibenzothiophene Based Electron Transport Materials. <i>Advances in Materials Physics and Chemistry</i> , 2012, 02, 219-225. | 0.3 | 6 |
| 15588 | Thiosemicarbazones Synthesized from Acetophenones: Tautomerism, Spectrometric Data, Reactivity and Theoretical Calculations. <i>International Journal of Analytical Mass Spectrometry and Chromatography</i> , 2019, 07, 19-34. | 0.7 | 5 |
| 15589 | Atomistic Simulations of Formation of Elementary Zr-I Systems. <i>Open Journal of Physical Chemistry</i> , 2011, 01, 104-108. | 0.1 | 6 |
| 15590 | Optical and Electronic Properties of Monomers of Eumelanin: A DFT and TD-DFT Computational Study. <i>Optics and Photonics Journal</i> , 2016, 06, 41-47. | 0.3 | 7 |
| 15591 | New Mechanism for the Reaction of Thianthrene Cation Radical Perchlorate with tert-Butyl Peroxide. <i>Bulletin of the Korean Chemical Society</i> , 2002, 23, 103-106. | 1.0 | 4 |
| 15592 | MP2 Basis Set Limit Binding Energy Estimates of Hydrogen-bonded Complexes from Extrapolation-oriented Basis Sets. <i>Bulletin of the Korean Chemical Society</i> , 2007, 28, 386-390. | 1.0 | 17 |
| 15593 | Uptake Effects of Two Electrons for Relative Stability and Atomic Structures of Carbon Cluster Isomers of C ₂₀ : ab initio Methods. <i>Bulletin of the Korean Chemical Society</i> , 2009, 30, 445-448. | 1.0 | 4 |
| 15594 | Full Geometry Optimizations of Bond-Stretch Isomers of C ₂₀ +Fullerene Dication by the Hybrid Density Functional B3LYP Methods. <i>Bulletin of the Korean Chemical Society</i> , 2011, 32, 277-280. | 1.0 | 3 |
| 15595 | Determination of Atomic Structures and Relative Stabilities of Diadduct Regioisomers of C ₂₀ X ₂ (X = H, F, Cl, Br, and OH) by the Hybrid Density-Functional B3LYP Method. <i>Bulletin of the Korean Chemical Society</i> , 2011, 32, 3372-3376. | 1.0 | 5 |
| 15596 | DFT Study for Substitution Patterns of C ₂₀ H ₁₈ X ₂ Regioisomers (X) <small>Tj ETQq0.0 0 rgBT/Overlock</small> | 1.0 | 7 |
| 15597 | Monohydrated Sulfuric and Phosphoric Acids with Different Hydrogen Atom Orientations: DFT and Ab initio Study. <i>Bulletin of the Korean Chemical Society</i> , 2012, 33, 1998-2004. | 1.0 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15598 | DFT Study of the Effect of the Li ₂ O Coating Pattern on the Volume and Band Gap of C ₂₀ Fullerene Cages. Bulletin of the Korean Chemical Society, 2013, 34, 365-366. | 1.0 | 3 |
| 15599 | Frontier Orbitals of Fifteen C ₂₀ H ₁₇ (OH) ₃ Regioisomers: Hybrid DFT B3LYP Study. Bulletin of the Korean Chemical Society, 2013, 34, 2403-2407. | 1.0 | 2 |
| 15600 | Stability and Interconversion of Acetylcholine Conformers. Bulletin of the Korean Chemical Society, 2014, 35, 2911-2916. | 1.0 | 3 |
| 15601 | Spin-orbit Effects on the Structure of Haloiodomethane Cations CH ₂ XI ⁺ (X=F, Cl, Br, and I). Bulletin of the Korean Chemical Society, 2014, 35, 775-782. | 1.0 | 4 |
| 15602 | Analysis of Nonclassical Fullerene C ₂₄ Regioisomers Encapsulating H ₂ O using Hybrid Density Functional Methods B3LYP and M06-2X. Bulletin of the Korean Chemical Society, 2014, 35, 899-904. | 1.0 | 1 |
| 15603 | Density Functional Study on [3+2]-Dipolar Cycloaddition Reaction of the N-heterocyclic Carbene Boryl Azide with Olefins. Bulletin of the Korean Chemical Society, 2014, 35, 1403-1408. | 1.0 | 1 |
| 15604 | mPW1PW91 Calculated Conformational Study of Calix[n]arene (n = 4,5,6): Hydrogen Bond. Journal of the Korean Chemical Society, 2009, 53, 640-652. | 0.2 | 1 |
| 15606 | DFT study of the decomposition reactions of nitroethyl benzoates catalyzed by the 1,3-dimethylimidazolium cation. Current Chemistry Letters, 2017, , 15-22. | 0.5 | 3 |
| 15608 | Identification of a bilirubin receptor that may mediate a component of cholestatic itch. ELife, 2019, 8, . | 2.8 | 86 |
| 15609 | Density Functional Theory Study on the Interaction of O ₂ Molecule with Cobalt ^{II} (6)Pyrrole Clusters. Japanese Journal of Applied Physics, 2011, 50, 055702. | 0.8 | 6 |
| 15610 | Why the Standard B3LYP/6-31G* Model Chemistry Should Not Be Used in DFT Calculations of Molecular Thermochemistry: Understanding and Correcting the Problem. Journal of Organic Chemistry, 2012, 77, 10824-10834. | 1.7 | 14 |
| 15611 | DFT Calculations of Mesembryanthemum nodiflorum Compounds as Corrosion Inhibitors of Aluminum. Physical Science International Journal, 2016, 12, 1-7. | 0.3 | 7 |
| 15612 | A Novel Prediction Model of Bandgap in Organic-Inorganic Hybrid Perovskites Based on a Simple Cluster Model Database. SSRN Electronic Journal, 0, , . | 0.4 | 0 |
| 15613 | A computational study of the reaction mechanism of 2,2-azobis(isobutyronitrile)-initiated oxidative cleavage of geminal alkenes. Organic and Biomolecular Chemistry, 2021, 19, 9483-9490. | 1.5 | 0 |
| 15614 | Understanding the behaviour of carnosine in aqueous solution: an experimental and quantum-based computational investigation on acid-base properties and complexation mechanisms with Ca ²⁺ and Mg ²⁺ . New Journal of Chemistry, 2021, 45, 20352-20364. | 1.4 | 7 |
| 15615 | <i>Ab initio</i> molecular dynamics simulations and experimental speciation study of levofloxacin under different pH conditions. Physical Chemistry Chemical Physics, 2021, 23, 24403-24412. | 1.3 | 2 |
| 15616 | Facile synthesis of hemiacetal ester-based dynamic covalent polymer networks combining fast reprocessability and high performance. Green Chemistry, 2021, 23, 9061-9070. | 4.6 | 14 |
| 15617 | The catalytic reaction mechanism of tyrosylprotein sulfotransferase-1. Physical Chemistry Chemical Physics, 2021, 23, 23850-23860. | 1.3 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 15618 | Tetra-substituted phthalocyanines bearing thiazolidine derivatives: synthesis, anticancer activity on different cancer cell lines, and molecular docking studies. Dalton Transactions, 2021, 50, 15778-15792. | 1.6 | 2 |
| 15619 | From molecular dynamics to quantum mechanics of misfolded proteins and amyloid-like macroaggregates applied to neurodegenerative diseases. Journal of Molecular Graphics and Modelling, 2022, 110, 108046. | 1.3 | 6 |
| 15620 | Substituent Effects and the Energetics of Noncatalyzed Aryl Halide Aminations: A Theoretical Investigation. ACS Omega, 2021, 6, 27216-27224. | 1.6 | 1 |
| 15621 | Local hybrid functionals augmented by a strong-correlation model. Journal of Chemical Physics, 2021, 155, 144101. | 1.2 | 12 |
| 15622 | A Novel Cyclopentadienone and its Ruthenium and Iron Tricarbonyl Complexes. European Journal of Inorganic Chemistry, 2021, 2021, 4832-4841. | 1.0 | 3 |
| 15623 | Raman microscopy-based quantification of the physical properties of intracellular lipids. Communications Biology, 2021, 4, 1176. | 2.0 | 15 |
| 15624 | Resolution of chemical shift anisotropy in ¹⁹ F ENDOR spectroscopy at 263 GHz/9.4 Å. Journal of Magnetic Resonance, 2021, 333, 107091. | 1.2 | 14 |
| 15625 | Bionic sunflower-like structure of polydopamine-confined NiFe-based quantum dots for electrocatalytic oxygen evolution reaction. Applied Catalysis B: Environmental, 2022, 302, 120833. | 10.8 | 25 |
| 15626 | a-PET and Weakened Triplet-Triplet Annihilation Self-Quenching Effects in Benzo-21-Crown-7-Functionalized Diiodo-BODIPY. ACS Omega, 2021, 6, 28356-28365. | 1.6 | 3 |
| 15627 | Stacked but not Stuck: Unveiling the Role of π - π^* Interactions with the Help of the Benzofuran-Formaldehyde Complex. Angewandte Chemie - International Edition, 2022, 61, . | 7.2 | 15 |
| 15628 | The Role of Structural Flexibility in Plasmon-Driven Coupling Reactions: Kinetic Limitations in the Dimerization of Nitro-Benzenes. Advanced Materials Interfaces, 2021, 8, 2101344. | 1.9 | 8 |
| 15629 | The Relationship between Enzyme Conformational Change, Proton Transfer, and Phosphoryl Transfer in β -Phosphoglucomutase. ACS Catalysis, 2021, 11, 12840-12849. | 5.5 | 7 |
| 15630 | Thermal Fluctuations in Conjugation and their Effect on Calculated Excitation Energies: A Case Study on the Astaxanthin Carotenoid. ChemPhotoChem, 2022, 6, . | 1.5 | 1 |
| 15631 | Nazarov Cyclizations Catalyzed by BINOL Phosphoric Acid Derivatives: Quantum Chemistry Struggles To Predict the Enantioselectivity. Journal of Organic Chemistry, 2022, 87, 1710-1722. | 1.7 | 5 |
| 15632 | Influence of non-adiabatic effects on linear absorption spectra in the condensed phase: Methylene blue. Journal of Chemical Physics, 2021, 155, 144112. | 1.2 | 13 |
| 15633 | A Bioinspired Adhesive-Integrated Agent Strategy for Constructing Robust Gas-Sensing Arrays. Advanced Materials, 2021, 33, e2106067. | 11.1 | 11 |
| 15634 | Performance of new exchange-correlation functionals in providing vertical excitation energies of metal complexes. Theoretical Chemistry Accounts, 2021, 140, 1. | 0.5 | 3 |
| 15635 | Do Double-Hybrid Exchange-Correlation Functionals Provide Accurate Chemical Shifts? A Benchmark Assessment for Proton NMR. Journal of Chemical Theory and Computation, 2021, 17, 6876-6885. | 2.3 | 34 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 15636 | Lowest Triplet and Singlet States in <i>N</i> -Methylacridone and <i>N,N</i> -Dimethylquinacridone: Theory and Experiment. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8777-8790. | 1.1 | 2 |
| 15637 | 5-IP7 is a GPCR messenger mediating neural control of synaptotagmin-dependent insulin exocytosis and glucose homeostasis. <i>Nature Metabolism</i> , 2021, 3, 1400-1414. | 5.1 | 13 |
| 15638 | Gas-Phase Fluorination of Hexagonal Boron Nitride. <i>Advanced Materials</i> , 2021, 33, e2106084. | 11.1 | 10 |
| 15639 | Activation of tetrahydrofuran with 2-((Fluoroalkyl)thio)Benzothiazolium reagents. <i>Tetrahedron</i> , 2021, 101, 132512. | 1.0 | 2 |
| 15640 | Ultrafast stimulated resonance Raman signatures of lithium polysulfides for shuttling effect characterization: An <i>ab initio</i> study. <i>Journal of Chemical Physics</i> , 2021, 155, 174301. | 1.2 | 2 |
| 15641 | Kernel Methods for Predicting Yields of Chemical Reactions. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2077-2092. | 2.5 | 27 |
| 15642 | Conformational Change in Molecular Crystals: Impact of Solvate Formation and Importance of Conformational Free Energies. <i>Crystal Growth and Design</i> , 2021, 21, 6924-6936. | 1.4 | 9 |
| 15643 | Comparing Properties of Common Bioinorganic Ligands with Switchable Variants of Cytochrome <i>c</i> . <i>Inorganic Chemistry</i> , 2021, , . | 1.9 | 2 |
| 15644 | Comparing Isoelectronic, Quadruple-Bonded Metalloporphyrin and Metalloporphyrin Dimers: Scalar-Relativistic DFT Calculations Predict a >1 eV Range for Ionization Potential and Electron Affinity. <i>ACS Physical Chemistry Au</i> , 2022, 2, 70-78. | 1.9 | 7 |
| 15645 | TDDFT and AIM evaluation of the effect of H and F abstraction from the calix[8]BODIPY molecule. <i>Computational and Theoretical Chemistry</i> , 2021, 1206, 113494. | 1.1 | 6 |
| 15646 | Fast and Accurate Electric Field Gradient Calculations in Molecular Solids With Density Functional Theory. <i>Frontiers in Chemistry</i> , 2021, 9, 751711. | 1.8 | 4 |
| 15647 | Highly accurate and constrained density functional obtained with differentiable programming. <i>Physical Review B</i> , 2021, 104, . | 1.1 | 21 |
| 15648 | Theory and Experiment Demonstrate that Sb(V)-Promoted Methane C-H Activation and Functionalization Outcompete Superacid Protonolysis in Sulfuric Acid. <i>Journal of the American Chemical Society</i> , 2021, 143, 18242-18250. | 6.6 | 8 |
| 15649 | Structural Elucidation, Aggregation, and Dynamic Behaviour of <i>N,N,N,N</i> -Copper(I) Schiff Base Complexes in Solid and in Solution: A Combined NMR, X-ray Spectroscopic and Crystallographic Investigation. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 4762-4775. | 1.0 | 8 |
| 15650 | Investigation of bis(perfluoro- <i>tert</i> -butoxy) halogenates(I/III). <i>Chemistry - A European Journal</i> , 2021, 27, 17676. | 1.7 | 1 |
| 15651 | Can (S)-Stereoisomers of Perezone and Its Derivatives Show Similar Activity to Its (R)-Stereoisomers? A Computational Characterization and Docking Study. <i>ChemistrySelect</i> , 2021, 6, 10974-10985. | 0.7 | 3 |
| 15652 | Oxygen vacancies on surface of the TiO ₂ fillers hinder Li ⁺ conduction in PEO all-solid-state electrolyte. <i>Ionics</i> , 2022, 28, 85-97. | 1.2 | 1 |
| 15653 | The Reaction N ₂ + CH ₃ CCH (Methylacetylene): A Combined Crossed Molecular Beams and Theoretical Investigation and Implications for the Atmosphere of Titan. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8846-8859. | 1.1 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15654 | Crystallography and QM/MM Simulations Identify Preferential Binding of Hydrolyzed Carbapenem and Penem Antibiotics to the L1 Metallo- β -Lactamase in the Imine Form. <i>Journal of Chemical Information and Modeling</i> , 2021, , . | 2.5 | 5 |
| 15655 | Experimental determination of the interaction potential between a helium atom and the interior surface of a C60 fullerene molecule. <i>Journal of Chemical Physics</i> , 2021, 155, 144302. | 1.2 | 15 |
| 15656 | Multi-state formulation of the frozen-density embedding quasi-diabatization approach. <i>Journal of Chemical Physics</i> , 2021, 155, 174104. | 1.2 | 4 |
| 15657 | A search for a DFT functional for actinide compounds. <i>Journal of Chemical Physics</i> , 2021, 155, 161103. | 1.2 | 6 |
| 15658 | Preparation, structure and dimerization of molecular tweezer: Cyanuric acid Core Based Flexible Symmetric linked Pthalimide moiety as a Heteroaromatic System. <i>Journal of Molecular Structure</i> , 2021, 1250, 131743. | 1.8 | 0 |
| 15659 | Stacked but not Stuck: Unveiling the Role of π π^* Interactions with the Help of the Benzofuran-Formaldehyde Complex. <i>Angewandte Chemie</i> , 2022, 134, e202113737. | 1.6 | 2 |
| 15660 | Electronic and Optical Properties of Polythiophene Molecules and Derivatives. <i>Crystals</i> , 2021, 11, 1292. | 1.0 | 12 |
| 15661 | Stable electrode-electrolyte interfaces constructed by fluorine- and nitrogen-donating ionic additives for high-performance lithium metal batteries. <i>Energy Storage Materials</i> , 2022, 45, 1-13. | 9.5 | 62 |
| 15662 | Ketone Incorporation Extends the Emission Properties of the Xanthene Scaffold Beyond 1000 nm. <i>Photochemistry and Photobiology</i> , 2022, 98, 325-333. | 1.3 | 18 |
| 15663 | Antiferromagnetic Exchange and Metal-Metal Bonding in Roussin's Black Sulfur and Selenium Salts. <i>Inorganic Chemistry</i> , 2021, 60, 16241-16255. | 1.9 | 1 |
| 15664 | Achieving a Favorable Activation of the C-F Bond over the C-H Bond in Five- and Six-Membered Ring Complexes by a Coordination and Aromaticity Dually Driven Strategy. <i>Organometallics</i> , 2021, 40, 3397-3407. | 1.1 | 11 |
| 15665 | Density Functional Theory-Inspired Design of Ir/P,S-Catalysts for Asymmetric Hydrogenation of Olefins. <i>Organometallics</i> , 2021, 40, 3424-3435. | 1.1 | 5 |
| 15666 | GdNi ₂ Sn ₂ electrocatalysts for active and selective ozone production. <i>AIChE Journal</i> , 2021, 67, e17486. | 1.8 | 8 |
| 15667 | Influence of fatty alcohol mixing ratios on physicochemical properties of stearyl polysorbate 60-water ternary system: Insights from experiments and computer simulations. <i>Colloid and Polymer Science</i> , 2021, 299, 1885-1900. | 1.0 | 5 |
| 15668 | Vibrational frequencies and intramolecular force constants for cisplatin: assessing the role of the platinum basis set and relativistic effects. <i>Journal of Molecular Modeling</i> , 2021, 27, 322. | 0.8 | 6 |
| 15669 | Fe-carbon hybrid composite interlayer for improved electrochemical performance of Li-S battery. <i>Electrochimica Acta</i> , 2022, 401, 139466. | 2.6 | 5 |
| 15670 | Electronic Structure Theory Calculations Using Modern Architectures: KNL vs Haswell. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6910-6917. | 2.3 | 1 |
| 15671 | High-level thermochemistry for the octasulfur ring: A converged coupled cluster perspective for a challenging second-row system. <i>Chemical Physics Impact</i> , 2021, 3, 100047. | 1.7 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15672 | Cytotoxic effect, spectroscopy, DFT, enzyme inhibition, and molecular docking studies of some novel mesitylamino propanols: Antidiabetic and anticholinergics and anticancer potentials. Journal of Molecular Liquids, 2021, 344, 117761. | 2.3 | 29 |
| 15673 | A Resonance Raman spectroscopic study on charge transfer enhancement in photosensitizers. Materials Today Advances, 2021, 12, 100180. | 2.5 | 1 |
| 15674 | Arylamination via ortho-fusion on an azo-appended pyridine carboxamide complex of copper(II). Journal of Organometallic Chemistry, 2021, 956, 122121. | 0.8 | 5 |
| 15675 | Hydroxyl on the filler surface promotes Li ⁺ conduction in PEO all-solid-state electrolyte. Solid State Ionics, 2021, 372, 115768. | 1.3 | 11 |
| 15678 | Quantum Chemical Calculations of Transition Metal Complexes. , 2003, , 361-380. | | 0 |
| 15679 | The Calculation of the Hyperfine Coupling Tensors of Biological Radicals. Progress in Theoretical Chemistry and Physics, 2003, , 239-265. | 0.2 | 1 |
| 15681 | Dimer Reference Embedded Atom Method (DR-EAM) and Its Application to Vacancy Formation Energy of FCC Metals. Yosetsu Gakkai Ronbunshu/Quarterly Journal of the Japan Welding Society, 2005, 23, 509-514. | 0.1 | 1 |
| 15682 | The SCF-LCAO-MO Method and Extensions. , 2006, , 348-390. | | 0 |
| 15683 | Recent Trends in Quantum Chemical Calculations for Surface-Molecule Interacting Systems. Hyomen Kagaku, 2007, 28, 150-159. | 0.0 | 0 |
| 15684 | A Density Functional Analysis on the Photoelectronic Spectra of Fe-Only Hydrogenase Analogues. E-Journal of Surface Science and Nanotechnology, 2007, 5, 148-151. | 0.1 | 0 |
| 15685 | Quadrupole coupling constants and isomeric Mössbauer shifts for halogen-containing gold, platinum, niobium, tantalum and antimony compounds. , 2008, , 547-556. | | 0 |
| 15686 | Density Functional Theory and Car-Parrinello Molecular Dynamics Methods. Advances in Photosynthesis and Respiration, 2008, , 487-499. | 1.0 | 1 |
| 15687 | Density Functional Calculation of the Structure and Electronic Properties of Cu _n O _n (n=1-4) Clusters. Lecture Notes in Computer Science, 2009, , 122-130. | 1.0 | 0 |
| 15688 | Electronic Structure Methods Based on Density Functional Theory. , 2009, , 478-488. | | 0 |
| 15690 | Polarization-dependent two-photon absorption of π -conjugated molecules. , 2010, , . | | 0 |
| 15691 | Density Functional Theory and the Kohn-Sham Equation. Springer Series in Solid-state Sciences, 2010, , 7-19. | 0.3 | 0 |
| 15692 | Selected applications of perturbed angular correlation of ^{137}Ba γ -rays (PAC) spectroscopy in biochemistry. , 2010, , 255-267. | | 0 |
| 15693 | Orbital-dependent Representation of Correlation Energy Functional. , 2010, , 165-176. | | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15694 | Theoretical Study of Cycloaddition Reactions of C ₆₀ on the Si(100)-2 \times 1 Surface. Bulletin of the Korean Chemical Society, 2010, 31, 1681-1688. | 1.0 | 2 |
| 15697 | TIMENmes: An Iron Nitride Complex. Springer Theses, 2012, , 19-51. | 0.0 | 0 |
| 15698 | A potential energy profile of the catalytic cycle of pyruvate decarboxylase. Natural Science, 2012, 04, 881-893. | 0.2 | 1 |
| 15699 | TIMENtol/3,5xyl: Unexpected Reactivity Resulting From Modifications of the Ligand Periphery. Springer Theses, 2012, , 53-83. | 0.0 | 0 |
| 15700 | Computational Studies on Effects of 1-(4-Chlorobenzylideneamino)-4-Phenyl-1H-Imidazol-2-Amine as an Anticancer Drug on DNA. International Journal of Bioscience, Biochemistry, Bioinformatics (IJBBB), 2012, , 126-130. | 0.2 | 0 |
| 15701 | The nature of the C \equiv As bonds in arsaalkynes: an atoms in molecules and electron localization function study. Highlights in Theoretical Chemistry, 2013, , 53-65. | 0.0 | 0 |
| 15702 | On the kinetics and thermodynamics of S \equiv X (X = H, CH ₃ , SCH ₃ , COCH ₃ , and CN) cleavage in the formation of self-assembled monolayers of alkylthiols on Au(111). Highlights in Theoretical Chemistry, 2013, , 99-109. | 0.0 | 0 |
| 15703 | Computational 19F NMR. 1. General features. Highlights in Theoretical Chemistry, 2013, , 41-52. | 0.0 | 0 |
| 15704 | Adsorption of successive layers of H ₂ molecules on a model copper surface: performances of second- to fifth-rung exchange-correlation functionals. Highlights in Theoretical Chemistry, 2013, , 281-289. | 0.0 | 0 |
| 15705 | [Zn ₁₀ ($\frac{1}{4}$ -S)($\frac{1}{4}$ -S) ₆ (Py) ₉ (SO ₄) ₃] as a molecular model of ZnS surfaces: an experimental and theoretical study. Highlights in Theoretical Chemistry, 2013, , 161-168. | 0.0 | 0 |
| 15706 | Quantum chemical study of self-doping PPV oligomers: spin distribution of the radical forms. Highlights in Theoretical Chemistry, 2014, , 87-93. | 0.0 | 0 |
| 15707 | Introduction to Vibrational Circular Dichroism. , 2012, , 1-12. | | 0 |
| 15708 | The Boron conundrum: the case of cationic clusters B_n^{+} with n = 2 \leq 20. Highlights in Theoretical Chemistry, 2014, , 71-85. | 0.0 | 0 |
| 15709 | The Mechanism of Formation of Glass-Ionomer Cement: A Theoretical Study. Modeling and Numerical Simulation of Material Science, 2013, 03, 149-154. | 0.5 | 1 |
| 15710 | Dancing multiplicity states supported by a carboxylated group in dicopper structures bonded to O ₂ . Highlights in Theoretical Chemistry, 2014, , 143-155. | 0.0 | 0 |
| 15711 | Computational Methods. Springer Theses, 2013, , 29-55. | 0.0 | 0 |
| 15712 | Organometallic copper I, II or III species in an intramolecular dechlorination reaction. Highlights in Theoretical Chemistry, 2014, , 105-110. | 0.0 | 0 |
| 15713 | Benchmarking the Performance of DHDFs for the Main Group Chemistry. Springer Briefs in Molecular Science, 2014, , 47-77. | 0.1 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15714 | An Overview of Modern Density Functional Theory. Springer Briefs in Molecular Science, 2014, , 1-24. | 0.1 | 0 |
| 15717 | Growth Mechanism, Energetics and CO Affinities of Vanadium Doped Gold Clusters, Au _n V with n = 1~20. , 2014, , 107-149. | | 0 |
| 15719 | Theoretical Methods. Springer Theses, 2014, , 9-34. | 0.0 | 0 |
| 15720 | Reduced Partition Function Ratio in the Frequency Complex Plane: A Mathematical Approach. Open Journal of Geology, 2014, 04, 654-664. | 0.1 | 1 |
| 15721 | Unidirectional Photo-induced Charge Separation and Thermal Charge Recombination of Cofacially Aligned Donor-Acceptor System Probed by Ultrafast Visible-Pump/Mid-IR-Probe Spectroscopy. Bulletin of the Korean Chemical Society, 2014, 35, 587-596. | 1.0 | 1 |
| 15722 | THE SCF-LCAO-MO METHOD AND EXTENSIONS. , 1993, , 350-391. | | 0 |
| 15724 | An Introduction to Water. , 2014, , 1-58. | | 0 |
| 15725 | Novel 1,3-dichalcogeno-2-phospholanes with an annelated 1,2-dicarba-closo-dodecaborane(12) Unit. Athens Journal of Sciences, 2014, 1, 83-96. | 0.1 | 0 |
| 15727 | Disclosure the Relationship "Structure Biology Activity" on the Basis of Conformational Analysis of the Brassinosteroid's Stereoisomers by the Molecular Modeling Methods. Mathematical Biology and Bioinformatics, 2014, 9, 386-395. | 0.1 | 0 |
| 15728 | The Quantum Chemical Calculations of Some Thiazole Derivatives. , 0, , . | | 2 |
| 15729 | Structure and Vibrational Spectra. , 2015, , . | | 0 |
| 15730 | GC/MS Analyses of Thiosemicarbazones Synthesized from Acetophenones: Thermal Decay and Mass Spectra Features. International Journal of Analytical Mass Spectrometry and Chromatography, 2015, 03, 1-13. | 0.7 | 1 |
| 15731 | 7.3.1 Group-IV semiconductor surfaces. , 2015, , 332-371. | | 0 |
| 15732 | Understanding the Exohedral Functionalization of Endohedral Metallofullerenes Metallofullerenes. Carbon Materials, 2015, , 67-99. | 0.2 | 0 |
| 15733 | Photoactive Semiconducting Oxides for Energy and Environment: Experimental and Theoretical Insights. , 2015, , 1-48. | | 0 |
| 15734 | A Theoretical Study on the Relevance of Protonated and Ionized Species of Methanimine and Methanol in Astrochemistry. Lecture Notes in Computer Science, 2016, , 296-308. | 1.0 | 1 |
| 15735 | NOVEL APPROACH TO MAKE HUGONIOT PREDICTIONS: QUANTUM MECHANICS/MOLECULAR DYNAMICS CALCULATIONS. International Journal of Energetic Materials and Chemical Propulsion, 2016, 15, 89-111. | 0.2 | 0 |
| 15738 | On the Chain Initiation Mechanism in the High Temperature Oxidation Process of C8 Alkane. , 2017, , . | | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15739 | Mechanistic Studies on Pd(OAc) ₂ -C ₆ H ₅ -catalyzed Meta-C-H Activation Reaction. Springer Theses, 2017, , 43-62. | 0.0 | 0 |
| 15740 | Mechanistic Studies on Pd(MPAA)-Catalyzed Meta- and Ortho-C-H Activation Reactions. Springer Theses, 2017, , 63-81. | 0.0 | 0 |
| 15741 | Silicate Nanoclusters: Understanding Their Cosmic Relevance from Bottom-Up Modelling. Challenges and Advances in Computational Chemistry and Physics, 2017, , 237-268. | 0.6 | 1 |
| 15742 | Density functional computational and X-ray studies on pharmaceutical compound 1-{3-[4-(4-fluorophenyl)piperazin-1-yl]propyl}-1H-indole. European Journal of Chemistry, 2017, 8, 1-7. | 0.3 | 3 |
| 15744 | Reviews in Infrared Spectroscopy and Computational Chemistry to Reveal Rhizospheric Interactions among Organic Acids, Oxyanions and Metal oxides: Fundamental Principles and Spectrum Processing. Daehan Hwan'gyeong Gonghag Hoeji, 2017, 39, 426-439. | 0.4 | 0 |
| 15745 | Nanotubular-structured porous silicon. Series in Materials Science and Engineering, 2017, , 591-598. | 0.1 | 0 |
| 15746 | Development of the Divide-and-Conquer Based Single Reference Theory for Static Correlation Systems with Finite Temperature Scheme. Journal of Computer Chemistry Japan, 2018, 17, 212-214. | 0.0 | 0 |
| 15748 | Charge-assisted hydrogen bonding in three diaminobenzene salts. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 1725-1731. | 0.2 | 2 |
| 15750 | Density Functional Methods. Springer Theses, 2019, , 29-70. | 0.0 | 0 |
| 15751 | Gas-Phase Molecular Geometry. Springer Theses, 2019, , 111-123. | 0.0 | 0 |
| 15752 | A New Î³-Butenolide Glycoside from the Root of Styphnolobium japonicum. Heterocycles, 2019, 98, 1251. | 0.4 | 0 |
| 15757 | Vibrational spectra, normal coordinate analysis, and structure of keto form of acetylacetone. A DFT approach. Egyptian Journal of Chemistry, 2019, . | 0.1 | 0 |
| 15758 | 1,2,5,6-tetrakis(guanidino)naphthalenes: Electron Donors, Fluorescent Probes and Redox-Active Ligands. Chemistry - A European Journal, 2020, 26, 5834-5845. | 1.7 | 6 |
| 15759 | Embedded Mean-Field Theory for Solution-Phase Transition-Metal Polyolefin Catalysis. Journal of Chemical Theory and Computation, 2020, 16, 4226-4237. | 2.3 | 3 |
| 15760 | Nuclear quantum and H/D isotope effects on three-centered bonding diborane: Path integral molecular dynamics simulations. International Journal of Quantum Chemistry, 2020, 120, e26179. | 1.0 | 1 |
| 15761 | A DFT Study of Si Doped Graphene: Adsorption of Formaldehyde and Acetaldehyde. Turkish Computational and Theoretical Chemistry, 2020, 4, 39-48. | 0.5 | 1 |
| 15763 | Wirt-Gast-Komplexe von [bfu.bfu.bfu]: Vorhersage von Ionenselektivitäten mittels quantenchemischer Rechnungen XIII. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2020, 75, 769-775. | 0.3 | 1 |
| 15764 | New spiro-borane and spiro-borate derived from dipyrromethane and their H/D exchange properties. Polyhedron, 2020, 186, 114612. | 1.0 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15765 | Synthesis, characterization of a novel molecule containing imine group, investigation of its quantum chemical, molecular docking and ADME properties. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-11. | 2.0 | 1 |
| 15766 | Beyond Conformational Control: Effects of Noncovalent Interactions on Molecular Electronic Properties of Conjugated Polymers. <i>Jacs Au</i> , 2021, 1, 2182-2187. | 3.6 | 8 |
| 15767 | Liquid-phase sintering of lead halide perovskites and metal-organic framework glasses. <i>Science</i> , 2021, 374, 621-625. | 6.0 | 137 |
| 15768 | SSIPTools: Software and Methodology for Surface Site Interaction Point (SSIP) Approach and Applications. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5331-5335. | 2.5 | 6 |
| 15769 | Substituent Effects on the Basicity of Patriscabrin A and Lettucenin A: Evolution Favors the Aromatic?. <i>ACS Omega</i> , 2021, 6, 29685-29691. | 1.6 | 2 |
| 15770 | Computer-aided estimation of kinetic rate constant for degradation of volatile organic compounds by hydroxyl radical: An improved model using quantum chemical and norm descriptors. <i>Chemical Engineering Science</i> , 2022, 248, 117244. | 1.9 | 13 |
| 15771 | Doubly Polarized QM/MM with Machine Learning Chaperone Polarizability. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7682-7695. | 2.3 | 5 |
| 15772 | In-situ polymerized solid-state electrolytes with stable cycling for Li/LiCoO ₂ batteries. <i>Nano Energy</i> , 2022, 91, 106679. | 8.2 | 62 |
| 15773 | The Enzymatic Decarboxylation Mechanism of 5-Carboxy Uracil: A Comprehensive Quantum Chemical Study. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 96-104. | 2.3 | 1 |
| 15774 | Structure, reactions, and electronic spectra of the rare gas cyanohydrides and isocyanohydrides, HRgCN and HRgNC (Rg = Xe or Rn). <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2020, 53, 245102. | 0.6 | 0 |
| 15775 | STRUCTURE OF IONS AND THE ENERGY OF THEIR FORMATION IN SATURATED ALUMINUM TRIS-DIPIVALOYLMETHANATE VAPOR UPON ELECTRON IONIZATION. <i>Journal of Structural Chemistry</i> , 2020, 61, 1852-1864. | 0.3 | 0 |
| 15776 | Stereoselective Cyclopropanation of Arylmethylidenemalononitriles by 2,6-Dimethylquinoline: A Molecular Electron Density Theory Study. <i>Russian Journal of Organic Chemistry</i> , 2020, 56, 2171-2178. | 0.3 | 0 |
| 15777 | The Proton Dissociation of Bio-Protic Ionic Liquids: [AAE]X Amino Acid Ionic Liquids. <i>Molecules</i> , 2021, 26, 62. | 1.7 | 0 |
| 15778 | Theoretical Study on Aluminum Oxide Cluster Anions Al ₂ O _x ^{-x} (x=2-5) with Rhombus Structure. <i>ChemistrySelect</i> , 2020, 5, 15137-15147. | 0.7 | 0 |
| 15779 | On the Mechanism of Bioinspired Formation of Inorganic Oxides: Structural Evidence of the Electrostatic Nature of the Interaction between a Mononuclear Inorganic Precursor and Lysozyme. <i>Biomolecules</i> , 2021, 11, 43. | 1.8 | 4 |
| 15780 | Enhanced Synthesis of oxo-Verdazyl Radicals Bearing Sterically-and Electronically-Diverse C3-Substituents. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 10120-10138. | 1.5 | 6 |
| 15781 | Highly red-emissive salen ⁱⁱ indium complexes: impact of 4-amino-substitution on the photophysical properties. <i>Inorganic Chemistry Frontiers</i> , 2021, 9, 119-126. | 3.0 | 5 |
| 15782 | Adaptive aromaticity in 16-valence-electron metallazapentalenes. <i>Dalton Transactions</i> , 2021, 50, 16842-16848. | 1.6 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15783 | Rapid electrochemical recognition of trimethoprim in human urine samples using new modified electrodes (CPE/Ag/Au NPs) analysing tunable electrode properties: experimental and theoretical studies. <i>Analyst</i> , 2021, 146, 7653-7669. | 1.7 | 6 |
| 15784 | Blocking the dark state as sensing mechanism of 3-nitro-1,8-naphthalimide derivatives for detection of carbon monoxide in the living cells. <i>Dyes and Pigments</i> , 2022, 197, 109905. | 2.0 | 10 |
| 15785 | Prominent dual Z-scheme mechanism on phase junction WO ₃ /CdS for enhanced visible-light-responsive photocatalytic performance on imidacloprid degradation. <i>Separation and Purification Technology</i> , 2022, 281, 119863. | 3.9 | 76 |
| 15786 | In pursuit of the ideal chromoionophores (part II): The structure-property relationship for electrochemical signaling capacities of aza-12-crown-4 ethers substituted with an anthraquinone moieties. <i>Dyes and Pigments</i> , 2022, 197, 109891. | 2.0 | 1 |
| 15787 | High-voltage nickel-rich layered cathodes in lithium metal batteries enabled by a sulfolane / fluorinated ether/ fluoroethylene carbonate-based electrolyte design. <i>Journal of Power Sources</i> , 2022, 517, 230683. | 4.0 | 9 |
| 15788 | Experimental and Theoretical Investigations of the Chemotherapeutic Drug Capecitabine. <i>Journal of Molecular Structure</i> , 2022, 1250, 131577. | 1.8 | 2 |
| 15789 | Molecular description of charge transport in the IDIC non-fullerene acceptor for organic solar cells. <i>Computational Materials Science</i> , 2022, 202, 110978. | 1.4 | 5 |
| 15790 | Facile immobilization of ethylenediamine tetramethylene-phosphonic acid into UiO-66 for toxic divalent heavy metal ions removal: An experimental and theoretical exploration. <i>Science of the Total Environment</i> , 2022, 806, 150652. | 3.9 | 43 |
| 15791 | Dissociation limit in Kohn-Sham density functional theory. <i>Nonlinear Analysis: Theory, Methods & Applications</i> , 2022, 215, 112633. | 0.6 | 0 |
| 15792 | Boosting oxygen-reduction catalysis over mononuclear CuN ₂₊₂ moiety for rechargeable Zn-air battery. <i>Chemical Engineering Journal</i> , 2022, 430, 133105. | 6.6 | 12 |
| 15793 | Study on the reaction mechanism of CH ₂ O + NO ₂ transformed by PbO/SnO in double-base propellants through theoretical calculation and experiment. <i>Combustion and Flame</i> , 2022, 236, 111768. | 2.8 | 4 |
| 15794 | An effective strategy for waste oil deoxygenation and upgrading for hydrocarbon biofuels production: A computational and experimental investigation. <i>Journal of the Energy Institute</i> , 2022, 100, 109-119. | 2.7 | 5 |
| 15795 | Insights into the mechanism during viscosity reduction process of heavy oil through molecule simulation. <i>Fuel</i> , 2022, 310, 122270. | 3.4 | 27 |
| 15796 | Thermally activated delayed fluorescence materials with aggregation-induced emission properties: a QM/MM study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25789-25796. | 1.3 | 10 |
| 15797 | Probing the role of surface acid sites on the photocatalytic degradation of tetracycline hydrochloride over cerium doped CdS via experiments and theoretical calculations. <i>Dalton Transactions</i> , 2021, 50, 16620-16630. | 1.6 | 9 |
| 15798 | Mechanisms and Origins of Regioselectivities of Nickel-Catalyzed \hat{I}^2, \hat{I}^1 -Vinylarylation of Alkenyl Esters with Vinyl Triflates and Arylzinc Reagents. <i>Organic Chemistry Frontiers</i> , 0, , . | 2.3 | 2 |
| 15799 | Aminopolycarboxylates in trivalent f-element separations. <i>Fundamental Theories of Physics</i> , 2021, 60, 1-162. | 0.1 | 2 |
| 15800 | Synthesis, structural characterization, thermal behaviour and antimicrobial activity of copper, cadmium and zinc chelates of traizole-thiole ligand in comparison with theoretical molecular orbital calculations. <i>Egyptian Journal of Chemistry</i> , 2019, . | 0.1 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15801 | Recent Developments in Density Functional Approximations. , 2020, , 213-226. | | 3 |
| 15802 | A Theoretical Investigation of the Reaction Between Glycolaldehyde and H ⁺ and Implications for the Organic Chemistry of Star Forming Regions. Lecture Notes in Computer Science, 2020, , 730-743. | 1.0 | 0 |
| 15804 | In silico decryption of serotoninâ€™receptor binding: local non-covalent interactions and long-range conformational changes. RSC Advances, 2020, 10, 37995-38003. | 1.7 | 1 |
| 15805 | Enzymatic Methane Hydroxylation: sMMO and pMMO. , 2020, , 45-73. | | 0 |
| 15807 | Intermolecular interaction energies and magnetic properties of spin-isolated multinuclear Cu ^{II} complexes. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 166-176. | 0.5 | 2 |
| 15810 | Establishing the accuracy of density functional approaches for the description of noncovalent interactions in ionic liquids. Physical Chemistry Chemical Physics, 2021, 23, 25558-25564. | 1.3 | 5 |
| 15811 | Diboron-controlled product selectivity switch in copper-catalyzed decarboxylative substitutions of alkynyl cyclic carbonates. Organic Chemistry Frontiers, 2021, 8, 6950-6961. | 2.3 | 3 |
| 15813 | Mechanism Investigation of Temperature Dependent Growth and Etching Process of GeCl ₄ on SiGe Surface: ab-initio Study. , 2021, , . | | 0 |
| 15814 | Vapor Pressure and Thermodynamics of L-Tryptophan Sublimation. Russian Journal of General Chemistry, 2021, 91, 1938-1945. | 0.3 | 6 |
| 15815 | The first-principles study of BC ₃ nanosheet as the delivery vehicle for 6-mercaptopurine drug. Molecular Physics, 2022, 120, . | 0.8 | 6 |
| 15816 | The ϵ -MD method to calculate NMR shift including effects due to conformational dynamics: The ^{31}P NMR shift in DNA . Journal of Computational Chemistry, 2022, 43, 132-143. | 1.5 | 5 |
| 15817 | Accurate Quantum Chemical Prediction of Gas-Phase Anion Binding Affinities and Their Structure-Binding Relationships. Journal of Physical Chemistry A, 2021, 125, 9838-9851. | 1.1 | 9 |
| 15818 | Characterization of oxorhenium(V) complexes with a benzyldithiocarbamate ligand: synthesis, spectroscopic and DFT analysis. Journal of Molecular Structure, 2021, , 131875. | 1.8 | 0 |
| 15819 | New Role for Radical SAM Enzymes in the Biosynthesis of Thio(seleno)oxazole RiPP Natural Products. Biochemistry, 2021, 60, 3347-3361. | 1.2 | 11 |
| 15820 | The Role of Thermodynamically Stable Configuration in Enhancing Crystallographic Diffraction Quality of Flexible MOFs. IScience, 2021, 24, 103398. | 1.9 | 1 |
| 15821 | Prediction of reaction mechanism for OH radical-mediated phenol oxidation using quantum chemical calculation. Chemosphere, 2022, 291, 132763. | 4.2 | 15 |
| 15822 | Rechargeable magnesium batteries enabled by conventional electrolytes with multifunctional organic chloride additives. Energy Storage Materials, 2022, 45, 1120-1132. | 9.5 | 40 |
| 15824 | X-ray absorption spectroscopy of small copper-oxide cluster ions for analyses of Cu oxidation state and Ar complexation: CuOAr ⁺ and Cu ₂ O ₂ ⁺ . Zeitschrift Fur Physikalische Chemie, 2021, 235, 213-224. | 1.4 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15825 | Theoretical Study of Circular Dichroism Spectra in the Vacuum-Ultraviolet. , 1999, , 93-119. | | 1 |
| 15826 | Theoretical Studies of Growth Reactions on Diamond Surfaces. , 2004, , 266-307. | | 2 |
| 15827 | Degradation of Polymers by O(3P) in Low Earth Orbit. , 2004, , 299-306. | | 0 |
| 15830 | Rotational States of Adsorbed H ₂ on Fe(OH) ₃ Molecule. Journal of the Physical Society of Japan, 2020, 89, 104601. | 0.7 | 0 |
| 15831 | Ionization and dissociation of benzene and aniline under deep ultraviolet laser irradiation. Chinese Journal of Chemical Physics, 2020, 33, 583-589. | 0.6 | 2 |
| 15832 | Density functional theory study on the adsorption of AsH ₃ gas molecule with monolayer (AlN) ₂₁ (including pristine, C, B doped and defective aluminium nitride sheet). IOP Conference Series: Materials Science and Engineering, 2020, 928, 072082. | 0.3 | 2 |
| 15834 | SYNTHESIS, STRUCTURAL CHARACTERIZATION, cis-trans ISOMERISM, AND DFT STUDIES ON cis-BIS(N,N-DI-METHYL-N-2-BENZOYLTHIOUREATO) PALLADIUM(II). Journal of Structural Chemistry, 2020, 61, 1751-1759. | 0.3 | 4 |
| 15835 | Yeni Heterosiklik Azo Bileşikler: Sentez, Karakterizasyon ve DFT Hesaplamalar. SDU Journal of Science, 0, , . | 0.1 | 0 |
| 15836 | Synthesis and Biological Activity of N-(Indolyl)trifluoroacetamides Based on Substituted 6-Aminoindoles. Moscow University Chemistry Bulletin, 2020, 75, 382-387. | 0.2 | 3 |
| 15837 | Study on N-(4-Chlorobenzoyl) Fenamic Acid Crystal-Density Functional Theory Approach. Sensor Letters, 2020, 18, 825-841. | 0.4 | 0 |
| 15838 | A linear metal-metal bonded tri-iron single-molecule magnet. Chemical Communications, 2021, 57, 13357-13360. | 2.2 | 10 |
| 15839 | Early Thermal Decay of Energetic Hydrogen- and Nitro-Free Furoxan Compounds: The Case of DNTF and BTF. Physical Chemistry Chemical Physics, 2021, , . | 1.3 | 5 |
| 15840 | Polyaniline-based gas sensors: DFT study on the effect of side groups. Computational and Theoretical Chemistry, 2022, 1207, 113526. | 1.1 | 8 |
| 15841 | Can time-dependent double hybrid density functionals accurately predict electronic excitation energies of BODIPY compounds?. Computational and Theoretical Chemistry, 2022, 1207, 113531. | 1.1 | 9 |
| 15842 | D-π-D based pyrido-pyrazino[2,3-b]indole amines as blue-red fluorescent dyes: Photophysical, aggregation-induced emission, electrochemical and theoretical studies. Journal of Luminescence, 2022, 242, 118568. | 1.5 | 16 |
| 15843 | Molecular dynamics studies on separation of CO ₂ /CH ₄ by the ionic liquids encapsulated ZIF-8. Journal of Membrane Science, 2022, 644, 120117. | 4.1 | 6 |
| 15844 | The Effect of Dicarboxylic Acid Catalyst Structure on Hydrolysis of Cellulose Model Compound D-Cellobiose in Water. Current Organocatalysis, 2022, 9, 163-171. | 0.3 | 1 |
| 15845 | Interfacial layer rich in organic fluoride enabling stable cycling of high-voltage PEO-based solid-state lithium batteries. Electrochimica Acta, 2022, 404, 139617. | 2.6 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 15846 | Pd(II)-Catalyzed Synthesis of Benzocyclobutenes by \hat{I}^2 -Methylene-Selective C(sp ³) \hat{C} -H Arylation with a Transient Directing Group. <i>Journal of the American Chemical Society</i> , 2021, 143, 20035-20041. | 6.6 | 37 |
| 15847 | THz trapped ion model and THz spectroscopy detection of potassium channels. <i>Nano Research</i> , 2022, 15, 3825-3833. | 5.8 | 4 |
| 15848 | Quantitative Theoretical Study of Molecular and Chain-Level Conformational Properties of Poly(ferrocenyldimethylsilanes). <i>Macromolecules</i> , 0, , . | 2.2 | 0 |
| 15849 | Enhancing the Accuracy of Ab Initio Molecular Dynamics by Fine Tuning of Effective Two-Body Interactions: Acetonitrile as a Test Case. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10475-10484. | 1.1 | 4 |
| 15850 | Exploring the Effects of a Doping Silver Atom on Anionic Gold Clusters TM Reactivity with O ₂ . <i>Journal of Physical Chemistry A</i> , 2021, 125, 9995-10005. | 1.1 | 6 |
| 15851 | Bridge-Length- and Solvent-Dependent Charge Separation and Recombination Processes in Donor \hat{C} Bridge \hat{C} Acceptor Molecules. <i>Journal of Physical Chemistry B</i> , 2021, 125, 13279-13290. | 1.2 | 5 |
| 15852 | Stereoisomerism in Tetrametallic Propeller \hat{C} Like Complexes: A Solid \hat{C} State and Solution NMR Study on a Tetragallium(III) Derivative. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, . | 1.0 | 0 |
| 15853 | BSE49, a diverse, high-quality benchmark dataset of separation energies of chemical bonds. <i>Scientific Data</i> , 2021, 8, 300. | 2.4 | 9 |
| 15854 | Accurate ⁵⁷ Fe Mössbauer Parameters from General Gaussian Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7724-7731. | 2.3 | 3 |
| 15855 | Symmetry Dilemma of Doubly Hybrid Density Functionals for Equilibrium Molecular Property Calculations. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7745-7752. | 2.3 | 5 |
| 15856 | Efficiency of Thermally Activated Delayed Fluorescence Sensitized Triplet Upconversion Doubled in Three \hat{C} Component System. <i>Advanced Materials</i> , 2022, 34, e2103976. | 11.1 | 13 |
| 15857 | Solid-State ²⁰⁷ Pb NMR Spectroscopy and Relativistic Quantum Chemical Calculations of Red Pigments: Identification in Cultural Heritage Materials. <i>Applied Magnetic Resonance</i> , 2022, 53, 371-385. | 0.6 | 1 |
| 15858 | Photophysical properties of push \hat{C} pull type chromophores of aryl-substituted bipyridines in different solvents. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 425, 113687. | 2.0 | 0 |
| 15859 | A generalized hybrid scheme for multireference methods. <i>Journal of Chemical Physics</i> , 2021, 155, 204106. | 1.2 | 1 |
| 15860 | Electro-catazone treatment of ozone-resistant drug ibuprofen: Interfacial reaction kinetics, influencing mechanisms, and degradation sites. <i>Journal of Hazardous Materials Advances</i> , 2021, 4, 100023. | 1.2 | 7 |
| 15861 | Relativistic Four-Component DFT Calculations of Vibrational Frequencies. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10315-10320. | 1.1 | 2 |
| 15862 | Doping Approaches for Organic Semiconductors. <i>Chemical Reviews</i> , 2022, 122, 4420-4492. | 23.0 | 153 |
| 15863 | On-Surface Synthesis of Boroxine-Based Molecules. <i>Chemistry</i> , 2021, 3, 1401-1410. | 0.9 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15864 | Structures 4-n-propyl Piperazines as Non-Imidazole Histamine H3 Antagonists. <i>Materials</i> , 2021, 14, 7094. | 1.3 | 0 |
| 15865 | A benzaldehyde derivative obtained from <i>Hypoxylon truncatum</i> NBRC 32353 treated with hygromycin B. <i>Journal of Antibiotics</i> , 2021, , . | 1.0 | 1 |
| 15866 | Sulfonated melanin derivatives: theoretical evaluation of local reactivities and chemical structures. <i>Journal of Molecular Modeling</i> , 2021, 27, 362. | 0.8 | 2 |
| 15867 | Selective Production of 2-Butanol from Hydrogenolysis of Levulinic Acid Catalyzed by the Non-precious NiMn Bimetallic Catalyst. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 15603-15611. | 3.2 | 14 |
| 15868 | Accelerated dinuclear palladium catalyst identification through unsupervised machine learning. <i>Science</i> , 2021, 374, 1134-1140. | 6.0 | 63 |
| 15869 | Influence of a lipophilic edaravone on physical state and activity of antioxidant liposomes: An experimental and in silico study. <i>Colloids and Surfaces B: Biointerfaces</i> , 2022, 210, 112217. | 2.5 | 1 |
| 15870 | Assessing and rationalizing the performance of Hessian update schemes for reaction path Hamiltonian rate calculations. <i>Journal of Chemical Physics</i> , 2021, 155, 204112. | 1.2 | 1 |
| 15871 | Intra-Molecular Electrical Field Regulated Nonlinear Catalyst Charge Transfer in the Organic Conjugated Molecular System. <i>Catalysts</i> , 2021, 11, 1375. | 1.6 | 0 |
| 15872 | Higher-Energy Hexafluoroisopropanol $\cdot\hat{A}\cdot\hat{A}\cdot$ Water Isomer and Its Large Amplitude Motions: Rotational Spectra and DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10401-10409. | 1.1 | 4 |
| 15873 | Spontaneous exciton dissociation enables spin state interconversion in delayed fluorescence organic semiconductors. <i>Nature Communications</i> , 2021, 12, 6640. | 5.8 | 18 |
| 15874 | Predicting Pt-195 NMR Chemical Shift and $1J(195\text{Pt}-31\text{P})$ Coupling Constant for Pt(0) Complexes Using the NMR-DKH Basis Sets. <i>Magnetochemistry</i> , 2021, 7, 148. | 1.0 | 4 |
| 15875 | A global analysis of excited states: the global transition contribution grids. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1. | 0.5 | 1 |
| 15876 | Copper-Catalyzed Enantioselective C \hat{C} H Arylation between 2-Arylindoles and Hypervalent Iodine Reagents. <i>Organic Letters</i> , 2021, 23, 9246-9250. | 2.4 | 11 |
| 15877 | Benchmark calculations and error cancelations for bond dissociation enthalpies of X \hat{C} NO $\hat{2}$. <i>Defence Technology</i> , 2023, 22, 144-155. | 2.1 | 6 |
| 15878 | Reaction of Alkynyl- and Alkenyltrifluoroborates with Propargyldicobalt Cations: Alkynylation, Alkenylation, and Cyclopropanation Product Pathways. <i>Journal of Organic Chemistry</i> , 2021, , . | 1.7 | 0 |
| 15879 | Switching Pathways of Triplet State Formation by Twisted Intramolecular Charge Transfer. <i>Journal of Physical Chemistry B</i> , 2021, 125, 12518-12527. | 1.2 | 6 |
| 15880 | Halogen-Manipulated Interfacial Charge Transport of \hat{I} -Conjugated Molecule-Lead Halide Hybrids. <i>ACS Applied Energy Materials</i> , 0, , . | 2.5 | 4 |
| 15881 | Electrochemical oxidation of ferricyanide. <i>Scientific Reports</i> , 2021, 11, 23058. | 1.6 | 17 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15882 | Fused aromatic networks as a new class of gas hydrate inhibitors. <i>Chemical Engineering Journal</i> , 2022, 433, 133691. | 6.6 | 7 |
| 15883 | Quantum-Mechanical/Molecular-Mechanical (QM/MM) Simulations for Understanding Enzyme Dynamics. <i>Methods in Molecular Biology</i> , 2022, 2397, 227-248. | 0.4 | 2 |
| 15884 | From simple alkenes and CO ₂ to fluorinated carboxylic acids: computational studies and predictions. <i>European Journal of Organic Chemistry</i> , 2022, 2022, e202101243. | 1.2 | 2 |
| 15885 | Interactions of C ₂ H ₆ and C ₂ H ₄ with the homologous series [C _n MIM][BF ₄] ionic liquids at high pressure studied by in situ ATR-FTIR spectroscopy. <i>Journal of Molecular Liquids</i> , 2022, 348, 118082. | 2.3 | 6 |
| 15886 | Quantifying Solvophobic Effects in Organic Solvents Using a Hydrocarbon Molecular Balance. <i>Journal of Organic Chemistry</i> , 2022, 87, 1874-1878. | 1.7 | 10 |
| 15887 | Voltage selection of physisorbed or chemisorbed 4-cyanobenzoate on a nanostructured silver electrode and the dual electronic structure of charged metal- molecule hybrids. <i>Applied Surface Science</i> , 2022, 579, 152071. | 3.1 | 2 |
| 15888 | Study on the dispersion mechanism of the polycarboxylic acid dispersant for disperse dyes. <i>Journal of Molecular Liquids</i> , 2022, 349, 118140. | 2.3 | 14 |
| 15889 | Theoretical Studies on Bimetallic Salen Complexes Catalyzed Epoxide Hydration: Effects of Metal Centers, Substrates, and Ligands. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10155-10164. | 1.1 | 3 |
| 15890 | Evolution of the Nature of Excitons and Electronic Couplings in Hybrid 2D Perovskites as a Function of Organic Cation Conjugation. <i>Advanced Functional Materials</i> , 2022, 32, 2108662. | 7.8 | 15 |
| 15891 | Highly efficient absorption of methyl tert-butyl ether with ionic liquids. <i>Separation and Purification Technology</i> , 2022, 282, 120108. | 3.9 | 8 |
| 15892 | Hydrogen-bonded supramolecular assemblies of folic acid with simple hexoses. <i>Journal of Molecular Structure</i> , 2022, 1250, 131904. | 1.8 | 0 |
| 15893 | Temperature-Induced Change of Water Structure in Aqueous Solutions of Some Kosmotropic and Chaotropic Salts. <i>International Journal of Molecular Sciences</i> , 2021, 22, 12896. | 1.8 | 4 |
| 15894 | Phase Diagrams and Spectral Characteristics of Hydrofluorocarbon Hydrates: Insights from First-Principles Thermodynamics. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 16347-16355. | 3.2 | 3 |
| 15895 | Benchmarking the Computational Costs and Quality of Vibrational Spectra from Ab Initio Simulations. <i>Advanced Theory and Simulations</i> , 2022, 5, 2100293. | 1.3 | 8 |
| 15896 | Phosphine-oxide organic ligand improved Cu-based catalyst for acetylene hydrochlorination. <i>Applied Catalysis A: General</i> , 2022, 630, 118461. | 2.2 | 13 |
| 15897 | Electron Delocalization in Spectroelectrochemically and Computationally Characterized [Pt(<i>p</i> -BrC ₆ F ₄)NCH ₂ (Cl)NEt ₂)Cl(<i>py</i>)] ⁺ Formed by Electrochemical Oxidation of [Pt(^{II})(<i>p</i> -BrC ₆ F ₄)NCH ₂ (Cl)NEt ₂)Cl(<i>py</i>)]. <i>Inorganic Chemistry</i> , 2021, 60, 18889-18911. | 1.9 | 1 |
| 15898 | A New Indole Substituted Biphenyldiamine Derivative Schiff Base: A New Sensor Application for the Selective Detection of Hg(II) Ions. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2021, 47, 903-908. | 0.3 | 2 |
| 15899 | Comparison of thermoresponsive Diels-Alder linkers for the release of payloads from magnetic nanoparticles via hysteretic heating. <i>Jcis Open</i> , 2021, 4, 100034. | 1.5 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 15900 | Investigation on the Ionic Composition and Spectroscopic Properties of Molten NaF-AlF ₃ -Al ₂ O ₃ Salts at 1300 K. Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science, 2022, 53, 474-484. | 1.0 | 4 |
| 15901 | Comparison of quantum mechanics protocols during the evaluation of quantitative structure-retention relationships supported by genetic-algorithm multiple linear regression. Journal of Chromatography Open, 2021, 1, 100019. | 0.8 | 2 |
| 15902 | Ligand-controlled divergent dehydrogenative reactions of carboxylic acids via C-H activation. Science, 2021, 374, 1281-1285. | 6.0 | 64 |
| 15903 | Defect Formation, T-Atom Substitution and Adsorption of Guest Molecules in MSE-Type Zeolite Framework—DFT Modeling. Molecules, 2021, 26, 7296. | 1.7 | 4 |
| 15904 | Switching of easy-axis to easy-plane anisotropy in cobalt(II) complexes. Inorganic Chemistry Frontiers, 2021, 8, 5158-5168. | 3.0 | 12 |
| 15905 | The Q41R mutation in the HCV-protease enhances the reactivity towards MAVS by suppressing non-reactive pathways. Physical Chemistry Chemical Physics, 2022, 24, 2126-2138. | 1.3 | 1 |
| 15906 | Access to metastable [GeH ₂] _n materials via a molecular “bottom-up” approach. Dalton Transactions, 2021, 50, 17688-17696. | 1.6 | 2 |
| 15907 | Dissociation of HCl in water nanoclusters: an energy decomposition analysis perspective. Physical Chemistry Chemical Physics, 2021, 23, 26737-26749. | 1.3 | 1 |
| 15908 | Ultrafast and efficient energy transfer in a one- and two-photon sensitized rhodamine-BODIPY dyad: a perspective for broadly absorbing photocages. Physical Chemistry Chemical Physics, 2022, 24, 1795-1802. | 1.3 | 4 |
| 15909 | Accurate calculation of spin-state energy gaps in Fe(III) spin-crossover systems using density functional methods. Dalton Transactions, 2021, 50, 17635-17642. | 1.6 | 7 |
| 15910 | Frontier orbitals stability of nitroxyl organic radicals probed by means of inner shell resonantly enhanced valence band photoelectron spectroscopy. Physical Chemistry Chemical Physics, 2022, . . | 1.3 | 2 |
| 15911 | Mechanistic Study of Cu-Catalyzed Addition Reaction of Isocyanates. Chinese Journal of Organic Chemistry, 2021, 41, 4347. | 0.6 | 4 |
| 15912 | Auto-Oxygenated Porphyrin-Derived Redox Mediators for High-Performance Lithium Air-Breathing Batteries. Advanced Energy Materials, 2022, 12, 2103527. | 10.2 | 15 |
| 15913 | Influence of Ionic Coordination on the Cathode Reaction Mechanisms of Al/S Batteries. Journal of Physical Chemistry C, 2022, 126, 40-47. | 1.5 | 5 |
| 15914 | Electronic energy levels of porphyrins are influenced by the local chemical environment. RSC Advances, 2022, 12, 1361-1365. | 1.7 | 4 |
| 15915 | 1,5-Diaminotetrazole-4- <i>N</i> -oxide (SYX-9): a new high-performing energetic material with a calculated detonation velocity over 10 km s ⁻¹ . Journal of Materials Chemistry A, 2022, 10, 1876-1884. | 5.2 | 21 |
| 15916 | Unveiling the complexity of the dual gold(I) catalyzed intermolecular hydroamination of alkynes leading to vinylazoles. Molecular Catalysis, 2022, 518, 112090. | 1.0 | 1 |
| 15917 | Covalent organic frameworks: Design and applications in electrochemical energy storage devices. Informa-Materially, 2022, 4, . | 8.5 | 31 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15918 | Photoinduced transformation of (Bu ₄ N) ₂ [Pt(NO ₃) ₆] complex in the solid state. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 427, 113788. | 2.0 | 2 |
| 15919 | Phase changes of tris(glycinato)chromium(III) monohydrate crystal systematically studied by thermal analyses, XRPD, FTIR, and Raman combined with ab initio calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 271, 120883. | 2.0 | 2 |
| 15920 | Theoretical Investigations of State Specific Hydrogen Atom Transfer in 8-Formyl-7-hydroxy-4-methylcoumarin. <i>Asian Journal of Chemistry</i> , 2022, 34, 256-262. | 0.1 | 0 |
| 15922 | Computational peptidology approach to the study of the chemical reactivity and bioactivity properties of Aspergillipeptide D, a cyclopentapeptide of marine origin. <i>Scientific Reports</i> , 2022, 12, 506. | 1.6 | 2 |
| 15923 | Tungsten(<i>vi</i>) selenide tetrachloride, WSeCl ₄ synthesis, properties, coordination complexes and application of [WSeCl ₄ (Se ⁿ Bu ₂)] for CVD growth of WSe ₂ thin films. <i>Dalton Transactions</i> , 2022, 51, 2400-2412. | 1.6 | 5 |
| 15924 | Efficient and regioselective synthesis of dihydroxy-substituted 2-aminocyclooctane-1-carboxylic acid and its bicyclic derivatives. <i>Beilstein Journal of Organic Chemistry</i> , 2022, 18, 77-85. | 1.3 | 2 |
| 15925 | Vibronic Coupling Effect on the Vibrationally Resolved Electronic Spectra and Intersystem Crossing Rates of a TADF Emitter: 7-PhQAD. <i>Journal of Physical Chemistry A</i> , 2022, 126, 239-248. | 1.1 | 25 |
| 15926 | Hydrogen Bonds of C=S, C=Se and C=Te with C-H in Small-Organic Molecule Compounds Derived from the Cambridge Structural Database (CSD). <i>Crystal Structure Theory and Applications</i> , 2022, 11, 1-22. | 0.3 | 3 |
| 15927 | High Efficiency Non Fullerene Acceptors Developed by Machine Learning and Quantum Chemistry. <i>Advanced Science</i> , 2022, 9, e2104742. | 5.6 | 28 |
| 15928 | NMR Coupling Constants Based on the Bethe-Salpeter Equation in the GW Approximation. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1030-1045. | 2.3 | 17 |
| 15929 | Mechanism of diethylamine/DBU-catalyzed cycloaddition of azides to unsaturated aldehydes: A quantum mechanical investigation. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113593. | 1.1 | 4 |
| 15930 | Interaction of halomethane CH ₃ Z (Z= F, Cl, Br) with X ₁₂ Y ₁₂ (X= B, Al, Ga & Y= N, P, As) nanocages. <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113544. | 1.1 | 18 |
| 15931 | Computational insight into the quantum chemistry, interaction and adsorption energy of aminopolycarboxylic acid chelating agents towards metal cations. <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113579. | 1.1 | 3 |
| 15932 | Thermal hazards and initial decomposition mechanisms study of four tert-butyl organic peroxides combining experiments with density functional theory method. <i>Thermochimica Acta</i> , 2022, 708, 179142. | 1.2 | 14 |
| 15933 | s-Tetrazine donor-acceptor electrodeposited layer with properties controlled by doping anions generally considered as interchangeable. <i>Electrochimica Acta</i> , 2022, 405, 139788. | 2.6 | 3 |
| 15934 | Kinetics and molecular mechanism of the Schonberg rearrangement. <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113585. | 1.1 | 1 |
| 15935 | Peculiar behavior of the ester carbonyl vibrational modes in anisotropic aliphatic and semi-aromatic polyesters. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 269, 120710. | 2.0 | 3 |
| 15936 | Mechanistic investigation of RhB photodegradation under low power visible LEDs using a Pd-modified TiO ₂ /Bi ₂ O ₃ photocatalyst: Experimental and DFT studies. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 162, 110510. | 1.9 | 17 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15937 | Colloidal templating of highly ordered porous amidoxime-functionalized hydrogel for intelligent treatment of uranium contaminated water. <i>Chemical Engineering Journal</i> , 2022, 431, 134141. | 6.6 | 24 |
| 15938 | First-principles calculations of molecular adsorption on the surface of two-dimensional BCOH. <i>Chemical Physics</i> , 2022, 555, 111442. | 0.9 | 1 |
| 15939 | A π -donor-free TM chromophore with a silicon-based acceptor group for second order nonlinear optics. <i>Inorganica Chimica Acta</i> , 2022, 533, 120745. | 1.2 | 2 |
| 15940 | peri-N-amine-perylenes, with and without phenyl bridge: Photophysical studies and their OLED applications. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 426, 113710. | 2.0 | 3 |
| 15941 | Synthesis of novel 2,5-bis(substituted thio)-1,3,4-thiadiazoles by acid catalyzed intermolecular cyclization reactions of substituted dithiocarbazates as a possible 2019-nCoV main protease inhibitor. <i>Journal of Molecular Structure</i> , 2022, 1253, 132252. | 1.8 | 2 |
| 15942 | Structural, spectral, and photoreactivity properties of mono and polymetallated-2,2'-bipyridine ruthenium(II) complexes. <i>Inorganica Chimica Acta</i> , 2022, 533, 120771. | 1.2 | 4 |
| 15943 | Experimental and theoretical study of three newly-synthesized iminochalcones: An example of dual emission induced by polarity changes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 426, 113725. | 2.0 | 0 |
| 15944 | A Simulation Research on Diffusion Processes of Discharging Decomposition Products of C4F7N/CO2 in Gas Insulated Transmission Lines. , 2020, , . | | 1 |
| 15946 | Gas-Phase Thermochemistry of MX ₃ and M ₂ X ₆ (M = Sc, Y; X = F, Cl). <i>J. Phys. Chem. B</i> , 2020, 124, 17084-17095. | 1.9 | 6 |
| 15947 | KID Procedure Applied on the [(PY ₅ Me ₂)MoO] ⁺ Complex. <i>ACS Omega</i> , 2020, 5, 30549-30555. | 1.6 | 2 |
| 15950 | New Isoquinoline Alkaloids from <i>Paraphaeosphaeria sporulosa</i> F03, a Fungal Endophyte Isolated from <i>Paepalanthus planifolius</i> . <i>Planta Medica</i> , 2022, 88, 994-1003. | 0.7 | 3 |
| 15951 | A Highly Active In Situ Zn(CH ₃ COO) ₂ -NC Catalyst for the Acetoxylation of Acetylene. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 1313-1321. | 1.8 | 5 |
| 15952 | (E)-4-((4-Bromobenzylidene) Amino)-N-(Pyrimidin-2-yl) Benzenesulfonamide from 4-Bromobenzaldehyde and Sulfadiazine, Synthesis, Spectral (FTIR, UV-Vis), Computational (DFT, HOMO-LUMO, MEP, NBO, NPA). <i>J. Phys. Chem. B</i> , 2022, 126, 11371-11381. | 1.8 | 1 |
| 15953 | Chalcogen Bonding in the Molecular Dimers of WCh ₂ (Ch = S, Se, Te): On the Basic Understanding of the Local Interfacial and Interlayer Bonding Environment in 2D Layered Tungsten Dichalcogenides. <i>International Journal of Molecular Sciences</i> , 2022, 23, 1263. | 1.8 | 12 |
| 15954 | Narrowband Deep-Blue Multi-Resonance Induced Thermally Activated Delayed Fluorescence: Insights from the Theoretical Molecular Design. <i>Molecules</i> , 2022, 27, 348. | 1.7 | 3 |
| 15955 | Nuclear Magnetic Resonance-Based Quality Assessment of Vermont-Grown Saffron (<i>Crocus sativus</i>). <i>J. Phys. Chem. B</i> , 2022, 126, 11371-11381. | 1.3 | 0 |
| 15956 | Controlling the diversity of ion-induced fragmentation pathways by N-methylation of amino acids. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 941-954. | 1.3 | 3 |
| 15957 | Computational Study of the Rh/phanephos-Catalyzed Enantioselective [2+2+2] Cyclization of Enediyne, Affording Lactone-Fused Cyclohexadiene Bearing a Quaternary Bridgehead Carbon. <i>Bulletin of the Chemical Society of Japan</i> , 2022, 95, 221-229. | 2.0 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 15958 | Decay Processes in Cationic Alkali Metals in Microsolvated Clusters: A Complex Absorbing Potential Based Equation-of-Motion Coupled Cluster Investigation. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 807-816. | 2.3 | 4 |
| 15959 | Insight into the computational modeling and reaction mechanism of the catalytic cycle of benzyl-dichalcogenide compounds in capture and release of carbon dioxide. <i>Molecular Catalysis</i> , 2022, 517, 112045. | 1.0 | 0 |
| 15960 | Thermoelectric properties plus phonon and de Haas-van Alphen frequencies of hole/electron-doped In_3Sb_7 . <i>Scientific Reports</i> , 2022, 12, 663. | 1.6 | 4 |
| 15961 | Synthesis, Characterization, and Biological Activities of Novel Vanadium(IV) and Cobalt(II) Complexes. <i>ACS Omega</i> , 2022, 7, 4389-4404. | 1.6 | 29 |
| 15962 | Cholesky decomposition of complex two-electron integrals over GIAOs: Efficient MP2 computations for large molecules in strong magnetic fields. <i>Journal of Chemical Physics</i> , 2022, 156, 044115. | 1.2 | 17 |
| 15963 | A Dual-Surface Mechanism of Oxidant-Free Pyrrole Polymerization in the Two-Dimensional Titanium Carbide (MXene) Interlayer Nanospace. <i>Journal of Physical Chemistry C</i> , 2022, 126, 1316-1325. | 1.5 | 5 |
| 15964 | Mechanism of Fuel Gas Denitration on the KOH-Activated Biochar Surface. <i>Journal of Physical Chemistry A</i> , 2022, 126, 296-305. | 1.1 | 6 |
| 15965 | Formation of phenylacetylene and benzocyclobutadiene in the <i>ortho</i> -benzyne + acetylene reaction. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1869-1876. | 1.3 | 4 |
| 15966 | Mechanistic insights into the rhodium-catalyzed aryl C-H carboxylation. <i>Organic Chemistry Frontiers</i> , 2022, 9, 370-379. | 2.3 | 4 |
| 15967 | Theoretically elucidating high photoluminescence performance of dimethylacridan-based blue-color thermally activated delayed fluorescent materials. <i>New Journal of Chemistry</i> , 2022, 46, 3464-3471. | 1.4 | 7 |
| 15968 | Mechanistically Guided Workflow for Relating Complex Reactive Site Topologies to Catalyst Performance in C-H Functionalization Reactions. <i>Journal of the American Chemical Society</i> , 2022, 144, 1881-1898. | 6.6 | 15 |
| 15969 | Understanding the mechanism of interfacial interaction enhancing photodegradation rate of pollutants at molecular level: Intermolecular H interactions favor electrons delivery. <i>Journal of Hazardous Materials</i> , 2022, 430, 128386. | 6.5 | 39 |
| 15970 | Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. <i>Angewandte Chemie - International Edition</i> , 2022, 61, . | 7.2 | 19 |
| 15971 | Computational insights into different regioselectivities in the Ir-porphyrin-catalyzed C-H insertion reaction of quinoid carbene. <i>Organic Chemistry Frontiers</i> , 2022, 9, 1143-1151. | 2.3 | 2 |
| 15972 | Demystifying constructive strategies on designing functionalized lamellar Nb_2CT_x nanosheet membrane architectures under confined space. <i>Journal of Materials Chemistry A</i> , 2022, 10, 4200-4208. | 5.2 | 0 |
| 15973 | Mechanistic Studies of the Catalytic Reduction of CO_2 to CO: Efficient CO-Releasing Si- and Ge-Based Catalysts. <i>ACS Omega</i> , 2022, 7, 4694-4702. | 1.6 | 2 |
| 15974 | New rhodium(III)-ED3AP complex: Crystal structure, characterization and computational chemistry. <i>Journal of the Serbian Chemical Society</i> , 2022, 87, 561-573. | 0.4 | 0 |
| 15975 | Expanding the known structure space for RNA binding: a test of 2,5-diketopiperazine. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 606-612. | 1.5 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15976 | A DFT examination of the role of proximal boron functionalities in the <i>S</i> -alkylation of sulfenic acid anions. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 649-657. | 1.5 | 3 |
| 15977 | DFT Studies and Quantum Chemical Calculations of Benzoyl Thiourea Derivatives Linked with Morpholine and Piperidine for the Evaluation of Antifungal Activity. <i>Current Physical Chemistry</i> , 2022, 12, . | 0.1 | 0 |
| 15978 | Rapid predictions of the colour purity of luminescent organic molecules. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4785-4794. | 2.7 | 12 |
| 15979 | Intensifying strategy of ionic liquids for Pd-based catalysts in anthraquinone hydrogenation. <i>Catalysis Science and Technology</i> , 2022, 12, 1766-1776. | 2.1 | 3 |
| 15980 | Soft-wall ion transfer channel accurately predicts sterically hindered ion channel permeability. <i>Bulletin of the Korean Chemical Society</i> , 2022, 43, 514-522. | 1.0 | 0 |
| 15981 | Machine learning reveals key ion selectivity mechanisms in polymeric membranes with subnanometer pores. <i>Science Advances</i> , 2022, 8, eabl5771. | 4.7 | 45 |
| 15982 | Proton Affinity Values of Fentanyl and Fentanyl Analogues Pertinent to Ambient Ionization and Detection. <i>Journal of the American Society for Mass Spectrometry</i> , 2022, 33, 482-490. | 1.2 | 6 |
| 15983 | A DFT study on the cyclization-degradation mechanism for phenylmethylsiloxanes in thermal vacuum. <i>Polymer Degradation and Stability</i> , 2022, 195, 109802. | 2.7 | 4 |
| 15984 | Acetate Facilitated Nickel Catalyzed Coupling of Aryl Chlorides and Alkyl Thiols. <i>ACS Catalysis</i> , 2022, 12, 2233-2243. | 5.5 | 32 |
| 15985 | Nickel Phthalocyanines as Potential Aggregation-Induced Antibacterial Agents: Fenton-Like Pathways Driven by Near-Infrared Light. <i>ChemPhotoChem</i> , 2022, 6, . | 1.5 | 3 |
| 15986 | LibSC: Library for Scaling Correction Methods in Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 840-850. | 2.3 | 8 |
| 15987 | Conceptual DFT-Based Computational Peptidology, Pharmacokinetics Study and ADMET Report of the Veraguamides A-G Family of Marine Natural Drugs. <i>Marine Drugs</i> , 2022, 20, 97. | 2.2 | 10 |
| 15988 | Automated assessment of redox potentials for dyes in dye-sensitized photoelectrochemical cells. <i>Physical Chemistry Chemical Physics</i> , 2021, 24, 197-210. | 1.3 | 4 |
| 15989 | Bz-8HQ: a novel supramolecular fluorochrome exhibiting multiple stimuli-responsiveness. <i>New Journal of Chemistry</i> , 2021, 46, 385-397. | 1.4 | 1 |
| 15990 | Near-infrared emitting copper(<i>i</i>) complexes with a pyrazolylpyrimidine ligand: exploring relaxation pathways. <i>Dalton Transactions</i> , 2022, 51, 2898-2911. | 1.6 | 7 |
| 15991 | Suzuki-type cross-coupling of alkyl trifluoroborates with acid fluoride enabled by NHC/photoredox dual catalysis. <i>Chemical Science</i> , 2022, 13, 2584-2590. | 3.7 | 42 |
| 15992 | Infrared Spectroscopy and Photochemistry of Anthracoronene in Cosmic Water Ice. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 165-180. | 1.2 | 2 |
| 15993 | Access to axially chiral styrenes via a photoinduced asymmetric radical reaction involving a sulfur dioxide insertion. <i>Chem Catalysis</i> , 2022, 2, 164-177. | 2.9 | 53 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 15994 | New Light on an Old Story: Breaking Kasha's Rule in Phosphorescence Mechanism of Organic Boron Compounds and Molecule Design. <i>International Journal of Molecular Sciences</i> , 2022, 23, 876. | 1.8 | 1 |
| 15995 | Superior performance of the machine-learning GAP force field for fullerene structures. <i>Structural Chemistry</i> , 2022, 33, 505-510. | 1.0 | 5 |
| 15996 | Synthesis of chiral polycyclic N-heterocycles via gold-catalyzed 1,6-enyne cyclization/intramolecular nucleophilic addition. <i>Chemical Communications</i> , 2022, 58, 3043-3046. | 2.2 | 5 |
| 15997 | Representations and strategies for transferable machine learning improve model performance in chemical discovery. <i>Journal of Chemical Physics</i> , 2022, 156, 074101. | 1.2 | 11 |
| 15998 | A Closer Look at the Isomerization of 5-androstene-3,17-dione to 4-androstene-3,17-dione in Ketosteroid Isomerase. <i>Journal of Computational Biophysics and Chemistry</i> , 0, , 1-21. | 1.0 | 2 |
| 15999 | Optimization and design for the curing process of solid azide propellant: Influence of typical components on the curing reactions of PBT binders with TDI. <i>Journal of the Chinese Chemical Society</i> , 2022, 69, 419-439. | 0.8 | 1 |
| 16000 | Theoretical and Structural Understanding of the Different Factors Influencing the Formation of Multicomponent Crystals of 2,4-Dichlorophenoxyacetic Acid with N-heterocyclic Compounds. <i>Crystal Growth and Design</i> , 2022, 22, 1707-1719. | 1.4 | 5 |
| 16001 | The electronic structure of the metal-organic interface of isolated ligand coated gold nanoparticles. <i>Nanoscale Advances</i> , 2022, 4, 1599-1607. | 2.2 | 7 |
| 16002 | Benzotriazole Ultraviolet Stabilizers Promote Breast Cancer Cell Proliferation via Activating Estrogen-Related Receptors $\text{ER}\alpha$ and $\text{ER}\beta$ at Human-Relevant Levels. <i>Environmental Science & Technology</i> , 2022, 56, 2466-2475. | 4.6 | 9 |
| 16003 | Bi ₂ O ₃ /WO ₃ Composite: A Bifunctional Plasmonic Heterostructure for Detection and Degradation Pollutions in Wastewater. <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 0 |
| 16004 | Computational Scaling Relationships Predict Experimental Activity and Rate-Limiting Behavior in Homogeneous Water Oxidation. <i>Inorganic Chemistry</i> , 2022, 61, 2186-2197. | 1.9 | 3 |
| 16005 | Insights into H ₂ Activation and Styrene Hydrogenation by Nickel-Borane and Nickel-Alane Bifunctional Catalysts. <i>Organometallics</i> , 2022, 41, 259-269. | 1.1 | 1 |
| 16006 | Accurate predictions of the electronic excited states of BODIPY based dye sensitizers using spin-component-scaled double-hybrid functionals: a TD-DFT benchmark study. <i>RSC Advances</i> , 2022, 12, 1704-1717. | 1.7 | 11 |
| 16007 | Exploration of the Mechanism of the Dimerization of Hydroxymethylsilanetriol Using Electronic Structure Methods. <i>ACS Omega</i> , 2022, 7, 2661-2670. | 1.6 | 0 |
| 16008 | Post-spin crossing dynamics determine the regioselectivity in open-shell singlet biradical recombination. <i>Organic Chemistry Frontiers</i> , 0, , . | 2.3 | 3 |
| 16009 | Electronic excitations through the prism of mean-field decomposition techniques. <i>Journal of Chemical Physics</i> , 2022, 156, 061101. | 1.2 | 4 |
| 16010 | Roles of Small Molecules in the Stability and Sensitivity of CL-20-Based Host-Guest Explosives under Electric Fields: A Reactive Molecular Dynamics Study. <i>Journal of Physical Chemistry A</i> , 2022, 126, 286-295. | 1.1 | 4 |
| 16011 | Density functionals with asymptotic-potential corrections are required for the simulation of spectroscopic properties of materials. <i>Chemical Science</i> , 2022, 13, 1492-1503. | 3.7 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16012 | Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. <i>Angewandte Chemie</i> , 0, , . | 1.6 | 6 |
| 16013 | The quantum chemical solvation of indole: accounting for strong solute-solvent interactions using implicit/explicit models. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3357-3369. | 1.3 | 6 |
| 16014 | Nucleophilicity and Electrophilicity in the Gas Phase: Silane Hydricity. <i>Journal of Organic Chemistry</i> , 2022, 87, 1840-1849. | 1.7 | 2 |
| 16015 | Ion transport in ionic liquid/poly(vinylidene fluoride) system under electric fields: A molecular dynamics simulation. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 642, 128328. | 2.3 | 3 |
| 16016 | Supervised Machine Learning Algorithms for Predicting Rate Constants of Ozone Reaction with Micropollutants. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 8359-8367. | 1.8 | 12 |
| 16017 | Antiaromaticity-promoted radical anion stability in $\hat{\pm}$ -vinyl heterocyclics. <i>Organic Chemistry Frontiers</i> , 0, , . | 2.3 | 3 |
| 16018 | Role of the Alkali Metal Cation in the Early Stages of Crystallization of Halide Perovskites. <i>Chemistry of Materials</i> , 2022, 34, 1121-1131. | 3.2 | 13 |
| 16019 | Chiral <i>N</i> -triflylphosphoramidate-catalyzed asymmetric hydroamination of unactivated alkenes: a hetero-ene reaction mechanism. <i>Organic Chemistry Frontiers</i> , 2022, 9, 1649-1661. | 2.3 | 4 |
| 16020 | Interplay Between Applied Force and Radical Attack in the Mechanochemical Chain Scission of Poly(acrylic acid). <i>Journal of Physical Chemistry A</i> , 2022, 126, 521-528. | 1.1 | 2 |
| 16021 | Insight Into the Stability and Electronic and Optical Properties of N-Heterocyclic Carbene Analogues of Halogen/Phosphine-Protected Au ₁₃ Superatomic Clusters. <i>Journal of Physical Chemistry A</i> , 2022, 126, 536-545. | 1.1 | 8 |
| 16022 | Synthesis, electronic structures, and reactivity of mononuclear and dinuclear low-valent molybdenum complexes in iminopyridine and bis(imino)pyridine ligand environments. <i>Journal of Inorganic Biochemistry</i> , 2022, 230, 111744. | 1.5 | 2 |
| 16023 | Theoretical Perspective on the Sensing Mechanism of a Novel Fluorescent Probe for Nitramine Explosives: The Role of Radical Reactions. <i>Journal of Physical Chemistry A</i> , 2022, 126, 685-690. | 1.1 | 1 |
| 16024 | Effective and irreversible removal of radioactive barium ions in MOF-808 framework functionalized sulfonic acid groups. <i>Green Chemical Engineering</i> , 2022, 3, 405-412. | 3.3 | 8 |
| 16025 | Promising and efficient lignin degradation versatile strategy based on DFT calculations. <i>IScience</i> , 2022, 25, 103755. | 1.9 | 4 |
| 16026 | Insights into Ionic Liquids: From Z-Bonds to Quasi-Liquids. <i>Jacs Au</i> , 2022, 2, 543-561. | 3.6 | 42 |
| 16027 | Ab initio and DFT benchmark study for the calculations of isotopic shifts of fundamental frequencies for 2,3-dihydropyran. <i>Structural Chemistry</i> , 0, , 1. | 1.0 | 1 |
| 16028 | Probing chirality across the electromagnetic spectrum with the full semi-classical light-matter interaction. <i>Journal of Chemical Physics</i> , 2022, 156, 054113. | 1.2 | 4 |
| 16029 | Triggering the energy release in molecular solar thermal systems: Norbornadiene-functionalized trioxatriangulen on Au(111). <i>Nano Energy</i> , 2022, 95, 107007. | 8.2 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16030 | Quantum chemical studies on chelation in nano-bio conjugate between ZnO nanoparticles and cellular energy carrier molecules. <i>Materials Chemistry and Physics</i> , 2022, 279, 125744. | 2.0 | 3 |
| 16031 | Dynamics of electric field-controlled methotrexate delivery through membrane nanochannels. <i>Journal of Molecular Liquids</i> , 2022, 350, 118525. | 2.3 | 0 |
| 16032 | Electrostatic interaction assisted Ca-decorated C20 fullerene loaded to anti-inflammatory drugs to manage cardiovascular disease risk in rheumatoid arthritis patients. <i>Journal of Molecular Liquids</i> , 2022, 350, 118564. | 2.3 | 18 |
| 16033 | Co-hydrothermal carbonization of biomass and PVC for clean blast furnace injection fuel production: Experiment and DFT calculation. <i>Renewable Energy</i> , 2022, 187, 156-168. | 4.3 | 16 |
| 16034 | The simulation study of transport performance of HU drugs on functionalized graphene nanosheets based on the Density Functional Theory. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113604. | 1.1 | 2 |
| 16035 | Near-Infrared fluorescent unsymmetrical aza-BODIPYs: Synthesis, photophysics and TD-DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 271, 120898. | 2.0 | 3 |
| 16036 | In-situ probing the near-surface structural thermal stability of high-nickel layered cathode materials. <i>Energy Storage Materials</i> , 2022, 46, 90-99. | 9.5 | 24 |
| 16037 | Hydrogen atom abstraction mechanism for organic compound oxidation by acetylperoxyl radical in Co(II)/peracetic acid activation system. <i>Water Research</i> , 2022, 212, 118113. | 5.3 | 44 |
| 16038 | Effect of K-decoration on the generation and reduction of $N\langle mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e287" altimg="si144.svg">\langle mml:msub>\langle mml:mrow />\langle mml:mrow>\langle mml:mn>2\langle /mml:mn>\langle /mml:mrow>\langle /mml:msub>\langle /mml:math>O$ onto a biochar surface. <i>Fuel</i> , 2022, 316, 123148. | 3.4 | 6 |
| 16039 | The uptake performance and microscopic mechanism of inorganic-organic phosphorus hybrid amorphous hydroxyapatite for multiple heavy metal ions. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 640, 128384. | 2.3 | 5 |
| 16040 | On relaxation and vibrational dynamics in the thermodynamic states of a chiral smectogenic glass-former. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 4595-4612. | 1.3 | 8 |
| 16041 | Reorganization energies of flexible organic molecules as a challenging target for machine learning enhanced virtual screening. , 2022, 1, 147-157. | | 11 |
| 16042 | The role of silver carbonate as a catalyst in the synthesis of N-phenylbenzamide from benzoic acid and phenyl isocyanate: a mechanistic exploration. <i>Australian Journal of Chemistry</i> , 2022, , . | 0.5 | 3 |
| 16043 | A system for artificial light signal transduction via molecular translocation in a lipid membrane. <i>Chemical Science</i> , 2022, 13, 2487-2494. | 3.7 | 4 |
| 16044 | A New Organic-Inorganic Hybrid Compound: Synthesis, crystal structure, Hirshfeld surface analysis, vibrational, optical, magnetic properties and theoretical study. <i>Polyhedron</i> , 2022, 217, 115717. | 1.0 | 5 |
| 16045 | Effect of substituents on the crystal structure and thermal stability of N-phosphorylated iminophosphoranes. <i>Journal of Thermal Analysis and Calorimetry</i> , 0, , 1. | 2.0 | 0 |
| 16046 | Investigation of SERS and Electron Transport Properties of Oligomer Phenylacetyne-3 Trapped in Gold Junctions. <i>Nanomaterials</i> , 2022, 12, 571. | 1.9 | 0 |
| 16047 | The Exception that Proves the Rule: How Sodium Chelation Can Alter the Charge-Cell Binding Correlation of Fluorescein-Based Multimodal Imaging Agents. <i>ChemMedChem</i> , 2022, , . | 1.6 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16048 | Î ⁺ NO and the complexities of electron correlation in simple hydrogen clusters. <i>Journal of Chemical Physics</i> , 2022, 156, 094102. | 1.2 | 4 |
| 16049 | Towards Nitrogen-Rich Heteropolycycles: Synthesis of Octaazaperopyrenes (OAPP). <i>Chemistry - A European Journal</i> , 2022, 28, . | 1.7 | 13 |
| 16050 | Sensitivity of the electronic and magnetic structures of cuprate superconductors to density functional approximations. <i>Npj Computational Materials</i> , 2022, 8, . | 3.5 | 12 |
| 16051 | Dual aggregation in ground state and ground-excited state induced by high concentrations contributes to chlorophyll stability. <i>Food Chemistry</i> , 2022, 383, 132447. | 4.2 | 2 |
| 16052 | Counterintuitive Electrostatics upon Metal Ion Coordination to a Receptor with Two Homotopic Binding Sites. <i>Journal of the American Chemical Society</i> , 2022, 144, 2921-2932. | 6.6 | 3 |
| 16053 | Free Energy Profiles of Proton Transfer Reactions: Density Functional Benchmark from Biased Ab Initio Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2022, , . | 2.3 | 5 |
| 16054 | Vibrational Spectra and Molecular Vibrational Behaviors of Dibenzyl Disulfide, Dibenzyl Sulphide and Bibenzyl. <i>International Journal of Molecular Sciences</i> , 2022, 23, 1958. | 1.8 | 8 |
| 16055 | Formation of Catalytically Active Nanoparticles under Thermolysis of Silver Chloroplatinate(II) and Chloroplatinate(IV). <i>Molecules</i> , 2022, 27, 1173. | 1.7 | 3 |
| 16056 | Novel modified BODIPY-C60 as photosensitizer in photodynamic therapy. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113632. | 1.1 | 2 |
| 16057 | Oxidative desulfurization of dibenzothiophene over highly dispersed Mo-doped graphitic carbon nitride. <i>Chemical Papers</i> , 2022, 76, 3401-3412. | 1.0 | 12 |
| 16058 | Accurate redox potentials for solvents in Li-metal batteries and assessment of density functionals. <i>International Journal of Quantum Chemistry</i> , 2022, 122, . | 1.0 | 6 |
| 16059 | A Mechanistic Study of Thermal Decomposition of 1,1,2,2-Tetramethyldisilane Using Vacuum Ultraviolet Photoionization Time-of-Flight Mass Spectrometry. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1085-1093. | 1.1 | 4 |
| 16061 | Ultrafast Solution-Phase Photophysical and Photochemical Dynamics of Hexaiodobismuthate(III), the Heart of Bismuth Halide Perovskite Solar Cells. <i>Journal of Physical Chemistry B</i> , 2022, 126, 1254-1267. | 1.2 | 3 |
| 16062 | A Combined Spectroscopic and Computational Study on the Mechanism of Iron-Catalyzed Aminofunctionalization of Olefins Using Hydroxylamine Derived N=O Reagent as the Amino-Source and Oxidant. <i>Journal of the American Chemical Society</i> , 2022, 144, 2637-2656. | 6.6 | 29 |
| 16063 | Decomposition of the interaction energy of several flavonoids with Escherichia coli DNA Gyr using the SAPT (DFT) method: The relation between the interaction energy components, ligand structure, and biological activity. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2022, 1866, 130111. | 1.1 | 2 |
| 16064 | Green Catalytic Method for Hydrothiolation of Allylamines: An External Electric Field. <i>ACS Omega</i> , 2022, 7, 5782-5790. | 1.6 | 2 |
| 16065 | Vibrational Treatment of Hydroxylamine in Valence Coordinates. <i>Journal of Chemical Physics</i> , 2022, 156, 084306. | 1.2 | 1 |
| 16066 | Density Functional Theory Transformed into a One-Electron Reduced-Density-Matrix Functional Theory for the Capture of Static Correlation. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 1382-1388. | 2.1 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16067 | Highly Emissive Red Heterobimetallic Ir ^{III} /M ^I (M = Cu) Tj ETQq0.00 rgBT /Overlock Materials, 2022, 34, 1756-1769. | 3.2 | 16 |
| 16068 | Efficient Zn ²⁺ , Pb ²⁺ , and Ni ²⁺ removal using antifouling mixed matrix nanofiltration membrane with curcumin modified mesoporous Santa Barbara Amorphous-15 (Cur-SBA-15) filler. Journal of Environmental Chemical Engineering, 2022, 10, 107302. | 3.3 | 12 |
| 16069 | Insight into the Gd ^{III} -Pt Bond: Slow Magnetic Relaxation of a Heterometallic Gd ^{III} -Pt Complex. Bulletin of the Chemical Society of Japan, 2022, 95, 513-521. | 2.0 | 3 |
| 16070 | Innovative characterization of original green vanillin-derived Schiff bases as corrosion inhibitors by a synergic approach based on electrochemistry, microstructure, and computational analyses. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 641, 128540. | 2.3 | 24 |
| 16071 | DFT Case Study on the Comparison of Ruthenium-Catalyzed C ^H Allylation, C ^H Alkenylation, and Hydroarylation. ACS Omega, 2022, 7, 6133-6141. | 1.6 | 2 |
| 16072 | Molecular modelling aided catalyst design for PAO oils hydrofinishing. Journal of Molecular Liquids, 2022, 352, 118675. | 2.3 | 21 |
| 16073 | Experimental and theoretical investigation of corrosion inhibition effect of two piperazine-based ligands on carbon steel in acidic media. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 641, 128538. | 2.3 | 26 |
| 16074 | Barriers to predictive high-throughput screening for spin-crossover. Computational Materials Science, 2022, 206, 111161. | 1.4 | 9 |
| 16075 | Decoding the Structure of Non-Proteinogenic Amino Acids: The Rotational Spectrum of Jet-Cooled Laser-Ablated Thioproline. Molecules, 2021, 26, 7585. | 1.7 | 3 |
| 16076 | Geometrical, electrical, and energetic parameters of hetero-disubstituted cumulenes and polyynes in the presence and absence of the external electric field. Structural Chemistry, 2022, 33, 479-490. | 1.0 | 3 |
| 16077 | Enantioseparation of novel anti-inflammatory chiral sulfoxides with two cellulose dichlorophenylcarbamate-based chiral stationary phases and polar-organic mobile phase(s). Journal of Chromatography Open, 2021, 1, 100022. | 0.8 | 4 |
| 16078 | Competing Singlet Fission and Excimer Formation in Solid Fluorinated 1,3-Diphenylisobenzofurans. Journal of Physical Chemistry C, 2021, 125, 27058-27071. | 1.5 | 9 |
| 16079 | De Novo Calculation of the Charge Carrier Mobility in Amorphous Small Molecule Organic Semiconductors. Frontiers in Chemistry, 2021, 9, 801589. | 1.8 | 7 |
| 16080 | Designing Potential Donor Materials Based on DRCN5T with Halogen Substitutions: A DFT/TDDFT Study. International Journal of Molecular Sciences, 2021, 22, 13498. | 1.8 | 2 |
| 16081 | Cellulose-Based Environment-Friendly Smart Materials for Colorimetric and Fluorescent Detection of Cu ²⁺ / Fe ³⁺ Ions and Their Anti-Counterfeiting Applications. SSRN Electronic Journal, 0, , . | 0.4 | 0 |
| 16082 | Proton-phosphorous connectivities revealed by high-resolution proton-detected solid-state NMR. Physical Chemistry Chemical Physics, 2022, 24, 7768-7778. | 1.3 | 6 |
| 16083 | Density Functional Theory for Transition Metal Catalysis. , 2024, , 562-585. | | 0 |
| 16084 | Comparing London dispersion pnicto-gen ^{II} interactions in naphthyl-substituted dipnictanes. Dalton Transactions, 2022, 51, 5016-5023. | 1.6 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16085 | Phosphine oxides as NMR and IR spectroscopic probes for the estimation of the geometry and energy of PO ⁻ H ⁺ A hydrogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7121-7133. | 1.3 | 2 |
| 16086 | Rational Design, Synthesis, and Pharmacological Characterization of Dicarboxyl Curcuminoid Analogs with Improved Stability Against Lung Cancer Via ROS and ER Stress Mediated Cell Apoptosis and Pyroptosis. <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 0 |
| 16087 | Chemical Bonding in Homogenous Catalysis – Seen Through the Eyes of Vibrational Spectroscopy. , 2024, , 622-648. | | 0 |
| 16088 | First Order Hyper polarizability and Intramolecular Charge Transfer of N-Ethyl-N-(2-Hydroxyethyl)-4-(4-Nitrophenylazo) Aniline for Photonic Applications. <i>IOP Conference Series: Materials Science and Engineering</i> , 2022, 1219, 012035. | 0.3 | 1 |
| 16089 | Oxalate promoted iron dissolution of hematite <i>via</i> proton coupled electron transfer. <i>Environmental Science: Nano</i> , 2022, 9, 1770-1779. | 2.2 | 7 |
| 16090 | Assessment of time-dependent density functionals for the electronic excitation energies of organic dyes used in DSSCs. <i>New Journal of Chemistry</i> , 2022, 46, 7682-7694. | 1.4 | 7 |
| 16091 | Blue-red emitting materials based on a pyrido[2,3- <i>b</i>]pyrazine backbone: design and tuning of the photophysical, aggregation-induced emission, electrochemical and theoretical properties. <i>RSC Advances</i> , 2022, 12, 6888-6905. | 1.7 | 9 |
| 16092 | Detection of multi-reference character imbalances enables a transfer learning approach for virtual high throughput screening with coupled cluster accuracy at DFT cost. <i>Chemical Science</i> , 2022, 13, 4962-4971. | 3.7 | 9 |
| 16093 | Manipulating the spin crossover behaviour in a series of cyanide-bridged {FeII2FeII2} molecular squares through NCE ⁺ co-ligands. <i>Dalton Transactions</i> , 2022, 51, 5596-5602. | 1.6 | 8 |
| 16094 | Mechanism and origins of enantioselectivity of cobalt-catalyzed intermolecular hydroacylation/cyclization of 1,6-enynes with aldehydes. <i>Organic Chemistry Frontiers</i> , 0, , . | 2.3 | 8 |
| 16095 | Structure-gelation property relationships of phenolic glycosides of pentose sugars: pH dependent controlled release of curcumin. <i>Materials Advances</i> , 0, , . | 2.6 | 0 |
| 16096 | Relationships with oxygen balance and bond dissociation energies. <i>Theoretical and Computational Chemistry</i> , 2022, , 67-79. | 0.2 | 2 |
| 16097 | Experimental and theoretical study of novel aminobenzamide-aminonaphthalimide fluorescent dyads with a FRET mechanism. <i>RSC Advances</i> , 2022, 12, 6192-6204. | 1.7 | 6 |
| 16098 | Kinetics and mechanistic details of bulk ZnO dissolution using a thiol-imidazole system. <i>Chemical Science</i> , 2022, 13, 3208-3215. | 3.7 | 5 |
| 16099 | Noncovalent interactions induced self-association in anthraquinone-iron aqueous redox flow batteries. <i>Sustainable Energy and Fuels</i> , 2022, 6, 2045-2052. | 2.5 | 2 |
| 16100 | Palladium-catalyzed regio- and chemoselective double-alkoxycarbonylation of 1,3-diyne: a computational study. <i>Organic Chemistry Frontiers</i> , 2022, 9, 2697-2707. | 2.3 | 4 |
| 16101 | Effects of stearyl alcohol monolayer on the structure, dynamics and vibrational sum frequency generation spectroscopy of interfacial water. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7374-7386. | 1.3 | 6 |
| 16102 | A tricolor-switchable stimuli-responsive luminescent binuclear Cu(ⁱ) complex with switchable NH ⁻ O interactions. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 2305-2314. | 3.0 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16103 | Designing Organic/Inorganic Cathodes of MnO ₂ Half-Wrapped by Aromatic Polymers for High-Performance Aqueous Zinc-Ion Batteries. SSRN Electronic Journal, 0, , . | 0.4 | 0 |
| 16104 | Theoretical Insights into the Intermolecular Hydrogen Bond Effect on ESIHT Process in 2- α -Hydroxychalcone: A Combined DFT/TDDFT Study. Asian Journal of Chemistry, 2022, 34, 849-856. | 0.1 | 0 |
| 16105 | Cyclo[18]carbon including zero-point motion: ground state, first singlet and triplet excitations, and hole transfer. Physical Chemistry Chemical Physics, 2022, 24, 7779-7787. | 1.3 | 4 |
| 16106 | Intramolecular rhodium-catalysed [2 + 2 + 2] cycloaddition of linear chiral <i>N</i> -bridged triynes: straightforward access to fused tetrahydroisoquinoline core. Organic and Biomolecular Chemistry, 2022, 20, 2433-2445. | 1.5 | 2 |
| 16107 | Insight into the dual action mechanism of 3V-PPh ₃ polymers as carriers and ligands in the Rh/3V-PPh ₃ heterogeneous catalytic hydroformylation of ethylene to propionaldehyde. Physical Chemistry Chemical Physics, 2022, 24, 9673-9684. | 1.3 | 4 |
| 16108 | Study of the DNA binding mechanism and <i>in vitro</i> activity against cancer cells of iron(III) and aluminium(III) kojic acid derivative complexes. Dalton Transactions, 2022, , . | 1.6 | 2 |
| 16109 | General quantitative structure–property relationships and machine learning correlations to energetic material sensitivities. Theoretical and Computational Chemistry, 2022, , 139-156. | 0.2 | 1 |
| 16110 | Solvent-Free and Catalyst-Free Chemistry Enables Insertion of Alkenes Into σ Bonds. SSRN Electronic Journal, 0, , . | 0.4 | 0 |
| 16111 | Influence of the Lewis basicity hardness of crystallization solvents on the coordination sphere of the complex [Co(3,5-dinitrobenzoate-O, π) ₂]: crystallographic and theoretical analysis. CrystEngComm, 2022, 24, 2982-2991. | 1.3 | 2 |
| 16112 | Quantum simulations of thermally activated delayed fluorescence in an all-organic emitter. Physical Chemistry Chemical Physics, 2022, 24, 10101-10113. | 1.3 | 6 |
| 16113 | A combined crystallography and DFT study on ring-shaped Cucurbit[<i>n</i>]urils: structures, surface character, and host–guest recognition. RSC Advances, 2022, 12, 10014-10019. | 1.7 | 4 |
| 16114 | From six to eight π -electron bare rings of group-XIV elements and beyond: can planarity be deciphered from the “quasi-molecules” they embed?. Physical Chemistry Chemical Physics, 2022, 24, 8488-8507. | 1.3 | 5 |
| 16115 | Ion-pairs as a gateway to transmetalation: aryl transfer from boron to nickel and magnesium. Dalton Transactions, 2022, 51, 5699-5705. | 1.6 | 1 |
| 16116 | Fundamental electronic changes upon intersystem crossing in large aromatic photosensitizers: free base 5,10,15,20-tetrakis(4-carboxylatophenyl)porphyrin. Physical Chemistry Chemical Physics, 2022, 24, 7505-7511. | 1.3 | 6 |
| 16117 | Metallophilicity versus π – π Interactions: Argentophilicity in Porphyrin Dimer. Asian Journal of Chemistry, 2022, 34, 557-561. | 0.1 | 0 |
| 16118 | Can a Wanzlick-like equilibrium exist between dicoordinate borylenes and diborenes?. Chemical Science, 0, , . | 3.7 | 3 |
| 16119 | THEORETICAL STUDIES ON STRUCTURE-DIRECTING INTERACTIONS OF DIPHENYL N-(2-PYRAZINYLYL CARBONYL) PHOSPHORAMIDATE. Journal of Structural Chemistry, 2022, 63, 140-151. | 0.3 | 1 |
| 16120 | Charge-Transfer Excitations within Density Functional Theory: How Accurate Are the Most Recommended Approaches?. Journal of Chemical Theory and Computation, 2022, 18, 1646-1662. | 2.3 | 30 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16121 | Charge-Transfer Excitation within a Hybrid-(G)KS Framework through Cartesian Grid DFT. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1448-1457. | 1.1 | 3 |
| 16122 | Exciton Dynamics of a Diketo-Pyrrolopyrrole Core for All Low-Lying Electronic Excited States Using Density Functional Theory-Based Methods. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1838-1848. | 2.3 | 5 |
| 16123 | 2,7-Substituted <i>N</i> -Carbazole Donors on Tris(2,4,6-trichlorophenyl)methyl Radicals with High Quantum Yield. <i>Advanced Optical Materials</i> , 2022, 10, . | 3.6 | 15 |
| 16124 | Activating Energy Transfer Tunnels by Tuning Local Electronegativity of Conjugated Polymeric Backbone for High-Efficiency OLEDs with Low Efficiency Roll-Off. <i>Advanced Functional Materials</i> , 2022, 32, . | 7.8 | 17 |
| 16125 | HF Formation through Dissociative Electron Attachment—A Combined Experimental and Theoretical Study on Pentafluorothiophenol and 2-Fluorothiophenol. <i>International Journal of Molecular Sciences</i> , 2022, 23, 2430. | 1.8 | 6 |
| 16126 | Probing effect of solvation on photoexcited quadrupolar donor-acceptor-donor molecule via ultrafast Raman spectroscopy. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 69-76. | 0.6 | 1 |
| 16127 | Free Energy and Stacking of Eumelanin Nanoaggregates. <i>Journal of Physical Chemistry B</i> , 2022, 126, 1805-1818. | 1.2 | 8 |
| 16128 | Multiscale Study of the Charge Transport Properties of Silicone Rubber Oligomers. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1369-1377. | 1.1 | 4 |
| 16129 | Direct synthesis of dimethyl carbonate from methanol and carbon dioxide over nickel loaded ceria as improved catalysts. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2022, 135, 937-950. | 0.8 | 3 |
| 16130 | Relative molecular orientations in organic optoelectronic films probed via polarization-selected UV/IR mixed frequency ultrafast spectroscopy. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 95-103. | 0.6 | 2 |
| 16131 | Theoretical Calculations and Experiments on the Thermal Properties of Fluorinated Graphene and Its Effects on the Thermal Decomposition of Nitrate Esters. <i>Nanomaterials</i> , 2022, 12, 621. | 1.9 | 8 |
| 16132 | BN-Substitution in Dithienylpyrenes Prevents Excimer Formation in Solution and in the Solid State. <i>Journal of Physical Chemistry C</i> , 2022, 126, 4563-4576. | 1.5 | 5 |
| 16133 | Computational Chemistry Derivation of Cr, Mn, and La Hydroxide and Oxyhydroxide Thermodynamics. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1551-1561. | 1.1 | 2 |
| 16134 | C(sp ³)-H Amination Catalyzed by Ir(Me)-Porphyrin: A Computational Study. <i>Organometallics</i> , 2022, 41, 569-580. | 1.1 | 4 |
| 16135 | Crystallization of Lactose-Protein Solutions in the Presence of Flavonoids. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 2684-2694. | 2.4 | 4 |
| 16136 | Design of new visible light Pt photocatalyst based on the TDDFT study of properties of transition metal complexes. <i>Applied Organometallic Chemistry</i> , 0, , . | 1.7 | 0 |
| 16137 | Carbon K-edge x-ray emission spectroscopy of gas phase ethylenic molecules. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2022, 55, 044001. | 0.6 | 5 |
| 16138 | Hybrid Synthetic and Computational Study of an Optimized, Solvent-Free Approach to Curcuminoids. <i>ACS Omega</i> , 2022, 7, 7257-7277. | 1.6 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16139 | Electrochemistry Applied to the Evaluation of the Interaction between Coumarins and the Copper Metal Ion: An Experimental Study with a DFT-Based Analysis. <i>Journal of the Electrochemical Society</i> , 2022, 169, 026526. | 1.3 | 0 |
| 16140 | The reliability of the small-core lanthanide effective core potentials. <i>Theoretical Chemistry Accounts</i> , 2022, 141, 1. | 0.5 | 2 |
| 16141 | Nucleophilic Aromatic Substitution of 5-Bromo-1,2,3-triazines with Phenols. <i>Journal of Organic Chemistry</i> , 2022, 87, 2590-2600. | 1.7 | 4 |
| 16142 | Solvated Nuclearâ€“Electronic Orbital Structure and Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1340-1346. | 2.3 | 9 |
| 16143 | Complementary, Cooperative Ditopic Halogen Bonding and Electron Donor-Acceptor ĨĖĖ Complexation in the Formation of Cocrystals. <i>Molecules</i> , 2022, 27, 1527. | 1.7 | 5 |
| 16144 | Innovative Microstructural Transformation upon CO ₂ Supercritical Conditions on Metal-Nucleobase Aerogel and Its Use as Effective Filler for HPLC Biomolecules Separation. <i>Nanomaterials</i> , 2022, 12, 675. | 1.9 | 0 |
| 16145 | Structureâ€“Activity Relationship of N-Phenylthieno[2,3-b]pyridine-2-carboxamide Derivatives Designed as Forkhead Box M1 Inhibitors: The Effect of Electron-Withdrawing and Donating Substituents on the Phenyl Ring. <i>Pharmaceuticals</i> , 2022, 15, 283. | 1.7 | 4 |
| 16146 | Benchmark Study on the Calculation of ¹¹⁹ Sn NMR Chemical Shifts. <i>Inorganic Chemistry</i> , 2022, 61, 3903-3917. | 1.9 | 11 |
| 16147 | Approximate functionals in hypercomplex Kohnâ€“Sham theory. <i>Electronic Structure</i> , 2022, 4, 014011. | 1.0 | 3 |
| 16148 | High Level Electronic Structure Calculation of Molecular Solid-State NMR Shielding Constants. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2408-2417. | 2.3 | 4 |
| 16149 | Synthesis of a Novel and More Sustainable Cationic Bleach Activator, <i>N</i> -[4-(<i>N,N,N</i> -Triethylammoniumchloride-butanoyl) Butyrolactam, for Cotton: Optimization and Theoretical Limitations. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 4415-4424. | 3.2 | 1 |
| 16150 | Chemical reactions of oily sludge catalyzed by iron oxide under supercritical water gasification condition. <i>Frontiers of Chemical Science and Engineering</i> , 2022, 16, 886-896. | 2.3 | 11 |
| 16151 | Magnetic Interplay between <i>d</i> -Electrons of Openâ€“Shell Porphyrins and <i>d</i> -Electrons of Their Central Transition Metal Ions. <i>Advanced Science</i> , 2022, 9, e2105906. | 5.6 | 9 |
| 16152 | Iron(III) Complexes of a Hexadentate Thioether-Appended 2-Aminophenol Ligand: Redox-Driven Spin State Switchover. <i>Inorganic Chemistry</i> , 2022, 61, 5292-5308. | 1.9 | 3 |
| 16153 | Effects of Salt Concentration on the Water and Ion Self-Diffusion Coefficients of a Model Aqueous Sodium-Ion Battery Electrolyte. <i>Journal of Physical Chemistry B</i> , 2022, 126, 2256-2264. | 1.2 | 11 |
| 16154 | Possible Ribose Synthesis in Carbonaceous Planetesimals. <i>Life</i> , 2022, 12, 404. | 1.1 | 6 |
| 16155 | Quasi-Relativistic Calculation of EPR <i>g</i> Tensors with Derivatives of the Decoupling Transformation, Gauge-Including Atomic Orbitals, and Magnetic Balance. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2246-2266. | 2.3 | 16 |
| 16156 | <i>In Situ Transâ€“Cis</i> Isomerization of Naphthylvinylpyridine Ligand in a Zinc(II) Coordination Polymer: Liquid and Vapor Phase Sensing of Mutagenic Pollutants and Nitroexplosives. <i>ACS Applied Polymer Materials</i> , 2022, 4, 2841-2850. | 2.0 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16157 | A DFT study on the reaction mechanisms of the oxidation of ethylene mediated by technetium and manganese oxo complexes. <i>Journal of Molecular Modeling</i> , 2022, 28, 94. | 0.8 | 2 |
| 16158 | IR microfluidics for in situ sensing of molecular interfaces. , 2022, , . | | 1 |
| 16159 | Finite-field coupling via learning the charge response kernel. <i>Electronic Structure</i> , 2022, 4, 014012. | 1.0 | 6 |
| 16160 | Successive Diels–Alder Cycloadditions of Cyclopentadiene to [10]CPP C_{60} : A Computational Study. <i>Journal of Organic Chemistry</i> , 2022, 87, 5149-5157. | 1.7 | 6 |
| 16161 | Functionalising the gate dielectric of organic field-effect transistors with self-assembled monolayers: effect of molecular electronic structure on device performance. <i>Applied Physics A: Materials Science and Processing</i> , 2022, 128, 1. | 1.1 | 3 |
| 16162 | Investigation of Molecular Iridium Fluorides IrF _n (n = 1–6): A Combined Matrix Isolation and Quantum-Chemical Study. <i>Chemistry - A European Journal</i> , 2022, , e202104005. | 1.7 | 2 |
| 16163 | Hybrid functionals with local range separation: Accurate atomization energies and reaction barrier heights. <i>Journal of Chemical Physics</i> , 2022, 156, 104109. | 1.2 | 10 |
| 16164 | In situ photodeposition of platinum clusters on a covalent organic framework for photocatalytic hydrogen production. <i>Nature Communications</i> , 2022, 13, 1355. | 5.8 | 140 |
| 16165 | Counterion-Induced Aggregation of Metallocarboranes. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5735-5742. | 1.5 | 9 |
| 16166 | Long-Range Intramolecular Spin Coupling through a Redox-Active Bridge upon Stepwise Oxidations: Control and Effect of Metal Ions. <i>Inorganic Chemistry</i> , 2022, 61, 5270-5282. | 1.9 | 3 |
| 16167 | Single Excitation Energies Obtained from the Ensemble α -HOMO–LUMO Gap: Exact Results and Approximations. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2452-2458. | 2.1 | 14 |
| 16168 | Tuning the Hydrolytic Behavior of Hydroxyquinoline Derivatives for Anticorrosion Applications. <i>Chemistry of Materials</i> , 2022, 34, 2842-2852. | 3.2 | 5 |
| 16169 | Phase transformation of heat-resistant energetic material BDNAPM studied by Raman spectroscopy and X-ray diffraction. <i>Journal of Materials Science</i> , 2022, 57, 6115-6128. | 1.7 | 1 |
| 16170 | High-Level Ab Initio Predictions of Thermochemical Properties of Organosilicon Species: Critical Evaluation of Experimental Data and a Reliable Benchmark Database for Extending Group Additivity Approaches. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1729-1742. | 1.1 | 2 |
| 16171 | Systematic Improvability in Quantum Embedding for Real Materials. <i>Physical Review X</i> , 2022, 12, . | 2.8 | 14 |
| 16172 | Adenosine Triphosphate Disodium Modified Hole Transport Layer for Efficient Inverted Perovskite Solar Cells. <i>ChemNanoMat</i> , 2022, 8, . | 1.5 | 2 |
| 16173 | Synthesis of Heterobimetallic Gold(I) Palladium(II) Bis(acyclic diaminocarbene) Complexes via the Isonitrile Route. <i>Organometallics</i> , 2022, 41, 802-810. | 1.1 | 8 |
| 16174 | Multiply charged naphthalene and its C ₁₀ H ₈ isomers: bonding, spectroscopy, and implications in AGN environments. <i>Monthly Notices of the Royal Astronomical Society</i> , 2022, 512, 4669-4682. | 1.6 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16175 | Unoccupied electronic structure of actinide dioxides. <i>Physical Review B</i> , 2022, 105, . | 1.1 | 9 |
| 16176 | Relativistic Effects in Modeling the Ligand K-Edge X-ray Absorption Near-Edge Structure of Uranium Complexes. <i>Journal of Chemical Theory and Computation</i> , 2022, , . | 2.3 | 3 |
| 16177 | Adsorption-Induced Expansion of Graphene Oxide Frameworks with Covalently Bonded Benzene-1,4-diboronic Acid: Numerical Studies. <i>ACS Omega</i> , 2022, 7, 11980-11987. | 1.6 | 1 |
| 16178 | Trifluoromethyl Substituted Derivatives of Pyrazoles as Materials for Photovoltaic and Electroluminescent Applications. <i>Crystals</i> , 2022, 12, 434. | 1.0 | 7 |
| 16179 | Morphology and Intramolecular Interactions in <i>P(VDF-TrFE)</i> Electrospun Nanofibers Doped with Disperse Orange 3 Dye: A Joint Infrared Spectroscopy and Electron Microscopy Study. <i>ACS Omega</i> , 2022, 7, 10660-10673. | 1.6 | 0 |
| 16180 | Effects of Mechanical Deformation on the Opto-Electronic Responses, Reactivity, and Performance of Conjugated Polymers: A DFT Study. <i>Polymers</i> , 2022, 14, 1354. | 2.0 | 2 |
| 16181 | Proton Radiation Hardness of Organic Photovoltaics: An In-Depth Study. <i>Solar Rrl</i> , 0, , 2101037. | 3.1 | 3 |
| 16182 | Internal dynamics of methyl <i>p</i> -tolyl sulfoxide in the gas phase: Rotational spectroscopy and theoretical studies. <i>Journal of Chemical Physics</i> , 2022, 156, 154304. | 1.2 | 1 |
| 16183 | An orbital-based representation for accurate quantum machine learning. <i>Journal of Chemical Physics</i> , 2022, 156, 114101. | 1.2 | 11 |
| 16184 | Through-Space Conjugated Electron Transport Materials for Improving Efficiency and Lifetime of Organic Light-Emitting Diodes. <i>Advanced Science</i> , 2022, 9, e2200374. | 5.6 | 27 |
| 16185 | Dielectric-Optical Switches: Photoluminescent, EPR, and Magnetic Studies on Organic-Inorganic Hybrid (azetidinium) ₂ MnBr ₄ . <i>Inorganic Chemistry</i> , 2022, 61, 5626-5636. | 1.9 | 20 |
| 16186 | Calculation of Core-Excited and Core-Ionized States Using Variational Quantum Deflation Method and Applications to Photocatalyst Modeling. <i>ACS Omega</i> , 2022, 7, 10840-10853. | 1.6 | 2 |
| 16187 | Theoretical study of germanium nanoclusters: significance of surface passivation. <i>European Physical Journal Plus</i> , 2022, 137, 1. | 1.2 | 0 |
| 16188 | Determining the Energy Gap between the S ₁ and T ₁ States of Thermally Activated Delayed Fluorescence Molecular Systems Using Transient Fluorescence Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2507-2515. | 2.1 | 12 |
| 16189 | 2 <i>H</i> -Imidazol-2-one <i>O</i> -Oxide: A Criegee Intermediate from a ⁰ İ ² Singlet Ground-State Carbene. <i>Journal of the American Chemical Society</i> , 2022, 144, 5937-5944. | 6.6 | 9 |
| 16190 | Protonation-Dependent Sequencing of 5-Formylcytidine in RNA. <i>Biochemistry</i> , 2022, 61, 535-544. | 1.2 | 10 |
| 16191 | A descriptor for the structural stability of organic-inorganic hybrid perovskites based on binding mechanism in electronic structure. <i>Journal of Molecular Modeling</i> , 2022, 28, 80. | 0.8 | 8 |
| 16192 | Hydrogen Storage Performance of Preferentially Oriented Mg/rGO Hybrids. <i>Chemistry of Materials</i> , 2022, 34, 2963-2971. | 3.2 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16193 | QM/MM Molecular Dynamics Simulations Revealed Catalytic Mechanism of Urease. <i>Journal of Physical Chemistry B</i> , 2022, 126, 2087-2097. | 1.2 | 9 |
| 16194 | Unsymmetrical Thienopentalenes: Synthesis, Optoelectronic Properties, and (Anti)aromaticity Analysis. <i>ACS Omega</i> , 2022, 7, 8336-8349. | 1.6 | 8 |
| 16195 | Resorcylic Acid-Based AIEgens for Illuminating Endoplasmic Reticulum**. <i>Chemistry - A European Journal</i> , 2022, 28, . | 1.7 | 2 |
| 16196 | Vernier template synthesis of molecular knots. <i>Science</i> , 2022, 375, 1035-1041. | 6.0 | 31 |
| 16197 | Free and open source software for computational chemistry education. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2022, 12, . | 6.2 | 19 |
| 16198 | Quantification of molecular aromaticity as a predictive factor of astrophysical significance. <i>Astronomy and Astrophysics</i> , 2022, 662, A106. | 2.1 | 1 |
| 16199 | Predicting properties of periodic systems from cluster data: A case study of liquid water. <i>Journal of Chemical Physics</i> , 2022, 156, 114103. | 1.2 | 13 |
| 16200 | CIDER: An Expressive, Nonlocal Feature Set for Machine Learning Density Functionals with Exact Constraints. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2180-2192. | 2.3 | 11 |
| 16201 | Epoxidation and Late-Stage C-H Functionalization by P450 Tam1 Are Mediated by Variant Heme-Iron Oxidizing Species. <i>ACS Catalysis</i> , 2022, 12, 3731-3742. | 5.5 | 9 |
| 16202 | Experimental and theoretical investigation on the thermal isomerization reaction of triazolotriazines. <i>Journal of Physical Organic Chemistry</i> , 0, , . | 0.9 | 1 |
| 16203 | Binding of Arsenic by Common Functional Groups: An Experimental and Quantum-Mechanical Study. <i>Applied Sciences (Switzerland)</i> , 2022, 12, 3210. | 1.3 | 3 |
| 16204 | Effect of Substituents on the Photodynamic Action of Anthraquinones: EPR, Computational and <i>In Vitro</i> Studies. <i>Photochemistry and Photobiology</i> , 2022, 98, 1426-1433. | 1.3 | 6 |
| 16205 | Density Functional Theory Study of Carbamoyl-Substituted Dihydroazulene/Vinylheptafulvene Derivatives and Solvent Effects. <i>Journal of Physical Chemistry C</i> , 2022, 126, 4815-4825. | 1.5 | 1 |
| 16206 | Remarkable NH_3 absorption in metal-based deep eutectic solvents by multiple coordination and hydrogen-bond interaction. <i>AIChE Journal</i> , 2022, 68, . | 1.8 | 44 |
| 16207 | A Synthetic Analog of Resveratrol Inhibits the Proangiogenic Response of Liver Sinusoidal Cells during Hepatic Metastasis. <i>Biomolecules and Therapeutics</i> , 2022, 30, 162-169. | 1.1 | 0 |
| 16208 | Highly Selective Synthesis of Seven-Membered Azaspiro Compounds by a Rh(I)-Catalyzed Cycloisomerization/Diels-Alder Cascade of 1,5-Bisallenenes. <i>Journal of Organic Chemistry</i> , 2022, 87, 5279-5286. | 1.7 | 7 |
| 16209 | Effect of EDTA Complexation on the Kinetics and Thermodynamics of Uranium Redox Reactions Catalyzed by Pyrite: A Combined Electrochemical and Quantum-Mechanical Approach. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 830-846. | 1.2 | 5 |
| 16210 | Modeling the Conformational Preference of the Lignocellulose Interface and Its Interaction with Weak Acids. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2119-2126. | 1.1 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16211 | Mechanism, Stereoselectivity, and Role of O ₂ in Aza-Diels-Alder Reactions Catalyzed by Dinuclear Molybdenum Complexes: A Theoretical Study. <i>Inorganic Chemistry</i> , 2022, 61, 4714-4724. | 1.9 | 3 |
| 16212 | High Fe utilization efficiency and low toxicity of Fe ₃ C@FeO loaded biochar for removing of tetracycline hydrochloride in wastewater. <i>Journal of Cleaner Production</i> , 2022, 353, 131630. | 4.6 | 18 |
| 16213 | Synthesis, Characterization, Biological Activity and Molecular Docking Studies of Novel Organotin(IV) Carboxylates. <i>Frontiers in Pharmacology</i> , 2022, 13, 864336. | 1.6 | 17 |
| 16214 | Investigation the effect of Ī bridge and side chain on photovoltaic properties of benzodithiophene and quinoxaline based conjugated polymers. <i>European Polymer Journal</i> , 2022, 169, 111141. | 2.6 | 6 |
| 16215 | Polyphenolic Compounds from <i>Lespedeza bicolor</i> Protect Neuronal Cells from Oxidative Stress. <i>Antioxidants</i> , 2022, 11, 709. | 2.2 | 6 |
| 16216 | Structural and Biophysical Analysis of the Phytochelatin-Synthase-Like Enzyme from <i>Nostoc</i> sp. Shows That Its Protease Activity is Sensitive to the Redox State of the Substrate. <i>ACS Chemical Biology</i> , 2022, 17, 883-897. | 1.6 | 3 |
| 16217 | Theoretical study of nickel-catalyzed hydroalkylation of 3-pyrrolines: Origin of ligand-controlled regioselectivity. <i>Molecular Catalysis</i> , 2022, 522, 112238. | 1.0 | 3 |
| 16218 | Revisiting the hydroxylation phenomenon of SiO ₂ : a study through "hard-hard" and "soft-soft" interactions. <i>Journal of Molecular Modeling</i> , 2022, 28, 115. | 0.8 | 0 |
| 16219 | DFT Mechanistic Study of the Cyclopropanation of Styrene and Aryldiazodiacetate Catalyzed by Tris(pentafluorophenyl)borane. <i>ACS Omega</i> , 2022, 7, 12900-12909. | 1.6 | 1 |
| 16220 | BF ₃ -Catalyzed Diels-Alder Reaction between Butadiene and Methyl Acrylate in Aqueous Solution: An URVA and Local Vibrational Mode Study. <i>Catalysts</i> , 2022, 12, 415. | 1.6 | 3 |
| 16221 | Hydrolysis of [PtCl ₆] ²⁻ in Concentrated NaOH Solutions. <i>Inorganic Chemistry</i> , 2022, 61, 5926-5942. | 1.9 | 6 |
| 16222 | Aminopolycarboxylic Acids-Functionalized Chitosan-Based Composite Cryogels as Valuable Heavy Metal Ions Sorbents: Fixed-Bed Column Studies and Theoretical Analysis. <i>Gels</i> , 2022, 8, 221. | 2.1 | 14 |
| 16223 | Lattice dynamics of BaFe ₂ Se ₃ . <i>Journal of Physics Condensed Matter</i> , 2022, 34, 255402. | 0.7 | 2 |
| 16224 | Coherent Control of Molecular Dissociation by Selective Excitation of Nuclear Wave Packets. <i>Frontiers in Chemistry</i> , 2022, 10, 859095. | 1.8 | 4 |
| 16225 | Synthesis, crystal structure, computational, and molecular docking studies of bis {1,1'-[1,3,5-Trimethyl-1,3-phenylenebis(methylene)]di-1H-piperidinium}tetrabromide tri hydrate. <i>Molecular Crystals and Liquid Crystals</i> , 0, , 1-18. | 0.4 | 1 |
| 16226 | Machine learned calibrations to high-throughput molecular excited state calculations. <i>Journal of Chemical Physics</i> , 2022, 156, 134116. | 1.2 | 5 |
| 16227 | Tuning Catalyst-Free Photocontrolled Polymerization by Substitution: A Quantitative and Qualitative Interpretation. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3290-3296. | 2.1 | 2 |
| 16228 | Improving Results by Improving Densities: Density-Corrected Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2022, 144, 6625-6639. | 6.6 | 45 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 16229 | Exploring the inhibitory potential of <i>Saussurea costus</i> and <i>Saussurea involucreta</i> phytoconstituents against the Spike glycoprotein receptor binding domain of SARS-CoV-2 Delta (B.1.617.2) variant and the main protease (Mpro) as therapeutic candidates, using Molecular docking, DFT, and ADME/Tox studies. <i>Journal of Molecular Structure</i> , 2022, 1263, 133032. | 1.8 | 14 |
| 16230 | Monitoring Methionine Decarboxylase by a Supramolecular Tandem Assay. <i>Chemistry - an Asian Journal</i> , 2022, 17, . | 1.7 | 4 |
| 16231 | Rational synthesis of ruthenium-based metallo-supramolecular polymers as heterogeneous catalysts for catalytic transfer hydrogenation of carbonyl compounds. <i>Applied Catalysis B: Environmental</i> , 2022, 312, 121383. | 10.8 | 10 |
| 16232 | Effect of Electron Donating/Withdrawing Groups on Molecular Photoswitching of Functionalized Hemithioindigo Derivatives: a Computational Multireference Study. <i>ChemPhotoChem</i> , 2022, 6, . | 1.5 | 4 |
| 16233 | Enantioselective Addition of Remote Alkyl Radicals to Double Bonds by Photocatalytic Proton-Coupled Electron Transfer (PCET) Deconstruction of Unstrained Cycloalkanols. <i>Organic Letters</i> , 2022, 24, 3123-3127. | 2.4 | 8 |
| 16234 | Arene-ruthenium(II) complexes with tetracyclic oxime derivatives: synthesis, structure and antiproliferative activity against human breast cancer cells. <i>Inorganica Chimica Acta</i> , 2022, 535, 120879. | 1.2 | 10 |
| 16235 | Mitigation effect of novel bipyrazole ligand and its copper complex on the corrosion behavior of steel in HCl: Combined experimental and computational studies. <i>Chemical Physics Letters</i> , 2022, 795, 139532. | 1.2 | 10 |
| 16236 | Different effects of oxysterols on a model lipid raft "Langmuir monolayer study complemented with theoretical calculations. <i>Chemistry and Physics of Lipids</i> , 2022, 244, 105182. | 1.5 | 5 |
| 16237 | Investigation of reaction mechanisms of CO ₂ reduction to methanol by Ni-C ₈₀ and Co-Si ₆₀ catalysts. <i>Inorganic Chemistry Communication</i> , 2022, 139, 109358. | 1.8 | 1 |
| 16238 | Influence of structural and solvation factors on spectral properties and lipophilicity of iodo- and bromosubstituted zinc(II), cadmium(II) and boron(III) dipyrromethenates. <i>Dyes and Pigments</i> , 2022, 201, 110202. | 2.0 | 3 |
| 16239 | Analysis of the behavior of Sn ²⁺ and In ³⁺ ions in DES and in water: A theoretical approach. <i>Journal of Molecular Liquids</i> , 2022, 353, 118774. | 2.3 | 2 |
| 16240 | Molecular dynamics study on the aggregation behaviours of Platonic micelle in different NaCl solutions. <i>Journal of Molecular Liquids</i> , 2022, 353, 118828. | 2.3 | 3 |
| 16241 | Linking azoles to isoniazid via hydrazone bridge: Synthesis, crystal structure determination, antitubercular evaluation and computational studies. <i>Journal of Molecular Liquids</i> , 2022, 354, 118873. | 2.3 | 6 |
| 16242 | Zinc(II) and cobalt(II) complexes with unusual coordination of mixed imidazole-1,2,4-triazole ligand in a protonated cationic form. <i>Polyhedron</i> , 2022, 217, 115741. | 1.0 | 7 |
| 16243 | Insight into understanding the photo-chemical stability of bis-tridentate Ir(III) phosphors: A theoretical perspective. <i>Dyes and Pigments</i> , 2022, 201, 110191. | 2.0 | 4 |
| 16244 | Preparation of activated coke by carbonization, activation, ammonization and thermal treatment of sewage sludge and waste biomass for SO ₂ absorption applications. <i>Fuel Processing Technology</i> , 2022, 231, 107233. | 3.7 | 24 |
| 16245 | Cellulose-based environment-friendly smart materials for colorimetric and fluorescent detection of Cu ²⁺ /Fe ³⁺ ions and their anti-counterfeiting applications. <i>Chemical Engineering Journal</i> , 2022, 438, 135595. | 6.6 | 19 |
| 16246 | Non-adiabatic dynamics of Rydberg-excited diethylamine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 274, 121065. | 2.0 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16247 | Bi/Bi ₂ O ₃ /WO ₃ composite: A bifunctional plasmonic heterostructure for detection and degradation pollutions in wastewater. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 107643. | 3.3 | 7 |
| 16248 | Development of magnetic nanoparticles for the intracellular delivery of miR-148b in non-small cell lung cancer. <i>Biomedical Engineering Advances</i> , 2022, 3, 100031. | 2.2 | 9 |
| 16249 | Confocal Raman microscopic evidence for cyclic water Pentamer, at high temperatures in a supramolecular host of [Cu(cyclam)(N ₃) ₂] ₂ ·4H ₂ O. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 274, 121121. | 2.0 | 3 |
| 16250 | Adsorption of a wide variety of antibiotics on graphene-based nanomaterials: A modelling study. <i>Chemosphere</i> , 2022, 296, 134010. | 4.2 | 13 |
| 16251 | Theoretical study on the extraction behaviors of MoO ₄ ²⁻ with organophosphorous extractants. <i>Journal of Molecular Liquids</i> , 2022, 355, 118969. | 2.3 | 5 |
| 16252 | Sodium tert-butoxide as stable electrode material in aprotic electrolyte for high cycle stability organic sodium-ion batteries. <i>Journal of Power Sources</i> , 2022, 532, 231361. | 4.0 | 3 |
| 16253 | Hydrogen bonds enhanced composite polymer electrolyte for high-voltage cathode of solid-state lithium battery. <i>Nano Energy</i> , 2022, 96, 107105. | 8.2 | 44 |
| 16254 | Fluoroaromatic 2H-imidazole-based push-pull fluorophores: Synthesis, theoretical studies, and application opportunities as probes for sensing the pH in saliva. <i>Dyes and Pigments</i> , 2022, 202, 110251. | 2.0 | 7 |
| 16255 | Pyridyl anchored indolium dyes for the p-type dye sensitized solar cell. <i>Dyes and Pigments</i> , 2022, 202, 110244. | 2.0 | 7 |
| 16256 | Studies on the antibacterial activities and molecular mechanism of GyrB inhibitors by 3D-QSAR, molecular docking and molecular dynamics simulation. <i>Arabian Journal of Chemistry</i> , 2022, 15, 103872. | 2.3 | 3 |
| 16257 | Solvent polarizability modulated the electronic state of conjugated long-chain polyene molecules by DFT. <i>Journal of Molecular Liquids</i> , 2022, 356, 119047. | 2.3 | 2 |
| 16258 | Theoretical correction on the existing understanding for hydroper-oxymethyl formate dissociation in DME low temperature oxidation. <i>Combustion and Flame</i> , 2022, 241, 112065. | 2.8 | 2 |
| 16259 | The solid-liquid equilibrium behavior of 2,7-dihydroxynaphthalene in eleven organic solvents: Thermodynamic analysis and molecular simulation understanding. <i>Journal of Chemical Thermodynamics</i> , 2022, 170, 106781. | 1.0 | 2 |
| 16260 | Mechanisms behind multicolor tunable Near-Infrared triple emission in graphene quantum dots and ratio fluorescent probe for water detection. <i>Journal of Colloid and Interface Science</i> , 2022, 617, 182-192. | 5.0 | 48 |
| 16261 | Polymeric ionic liquid with carboxyl anchored on mesoporous silica for efficient fixation of carbon dioxide. <i>Journal of Colloid and Interface Science</i> , 2022, 618, 44-55. | 5.0 | 27 |
| 16262 | Electronic and steric factors affecting the ligands redistribution reaction of [Cu(2,2'-biquinoline)(PR ₃) ₂] ⁺ systems in fluid solutions. <i>Journal of Molecular Structure</i> , 2022, 1261, 132933. | 1.8 | 2 |
| 16263 | Hydrogen Complexes of 1,2-Naphthoquinone with Water Molecules in Aqueous Solution and Their Influence on Shifts of Absorption Bands. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2022, 47, 107-114. | 0.2 | 0 |
| 16264 | Photochemistry of 2,2-Dimethyl- and 2,2,3-Trimethyloxirane Radical Cations in Freon Matrices at 77 K. <i>Moscow University Chemistry Bulletin</i> , 2021, 76, 361-369. | 0.2 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16265 | Quantum Chemical Insight into Molecular Structure, Spectroscopic and Nonlinear Optical Studies on Methylene bis(dithiobenzoate). Optics and Spectroscopy (English Translation of Optika I) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 737 Td (| | |
| 16266 | Simulation of Gas Production Mechanisms in Shear Deformation of Medium-Rank Coal. ACS Omega, 2022, 7, 342-350. | 1.6 | 3 |
| 16267 | Isotope Effects on the Vaporization of Organic Compounds from an Aqueous Solution—Insight from Experiment and Computations. Journal of Physical Chemistry B, 2021, 125, 13868-13885. | 1.2 | 5 |
| 16268 | A Study of Factors Affecting Various Reactions of Thermal Decomposition of Ethyl Fluoroformate Using Ab Initio Quantum Mechanics Calculations. Russian Journal of Physical Chemistry A, 2021, 95, S307-S313. | 0.1 | 0 |
| 16269 | Acid-Catalyzed Esterification of Betaines: Theoretical Exploration of the Impact of the Carbon Chain Length on the Reaction Mechanism. Physchem, 2021, 1, 288-296. | 0.5 | 0 |
| 16270 | Pharmacokinetics and drug-likeness of antidiabetic flavonoids: Molecular docking and DFT study. PLoS ONE, 2021, 16, e0260853. | 1.1 | 50 |
| 16271 | High-Fidelity Dimerization of Xanthenyl Radicals and Dynamic Qualities of a Congested Ethane: Diethyl Dixanthenyl-9,9-dicarboxylate. European Journal of Organic Chemistry, 2022, 2022, . | 1.2 | 1 |
| 16272 | Understanding the Photocatalytic Reduction of CO ₂ with Heterometallic Molybdenum(V) Phosphate Polyoxometalates in Aqueous Media. ACS Catalysis, 2022, 12, 453-464. | 5.5 | 27 |
| 16273 | Methane and Acetylene Detection in Transformer Oil Based on Raman Spectroscopy. , 2021, , . | | 0 |
| 16274 | Perfluorination of Aromatic Compounds Reinforce Their van der Waals Interactions with Rare Gases: The Rotational Spectrum of Pentafluoropyridine-Ne. Molecules, 2022, 27, 17. | 1.7 | 3 |
| 16275 | Catalyst-Controlled Stereoselective Construction of Indole-Fused Heterocycles through Cycloadditions of Indolyl-Allenes: A Theoretical Investigation. Russian Journal of Physical Chemistry A, 2021, 95, 2567-2572. | 0.1 | 0 |
| 16276 | Charge transfer excitations and constrained density functional theory. Theoretical Chemistry Accounts, 2022, 141, 1. | 0.5 | 8 |
| 16277 | An Improved Synthesis of Bromotetrazole. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2022, 648, . | 0.6 | 0 |
| 16278 | Laser-induced fluorescence experimental spectroscopy and theoretical calculations of uranium monoxide. Chinese Physics B, 0, , . | 0.7 | 2 |
| 16279 | Theoretical Design of Blue-Color Phosphorescent Complexes for Organic Light-Emitting Diodes: Emission Intensities and Nonradiative Transition Rate Constants in Ir(ppy) ₂ (acac) Derivatives. Journal of Physical Chemistry A, 2021, 125, 10604-10614. | 1.1 | 0 |
| 16280 | Accelerating the Convergence of Self-Consistent Field Calculations Using the Many-Body Expansion. Journal of Chemical Theory and Computation, 2022, 18, 179-191. | 2.3 | 6 |
| 16281 | Artificial Bipolar Redox-Active Molecule for Symmetric Nonaqueous Redox Flow Batteries. ACS Sustainable Chemistry and Engineering, 2022, 10, 613-621. | 3.2 | 9 |
| 16282 | Electronic Energy and Local Property Errors at QTAIM Critical Points while Climbing Perdew's Ladder of Density-Functional Approximations. Journal of Chemical Theory and Computation, 2022, 18, 293-308. | 2.3 | 14 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16283 | Ethylene-Triggered Regioselectivity Switch of Dimethylbutadiene in Their Copolymerization: Formation of "Plastic" Rubber and Mechanism. <i>ACS Catalysis</i> , 2022, 12, 953-962. | 5.5 | 5 |
| 16284 | DFT study on the mechanisms of C-C cross coupling of C=C bonds catalyzed by iron complexes. <i>Applied Organometallic Chemistry</i> , 2022, 36, . | 1.7 | 6 |
| 16285 | Side-by-Side Comparison of Five Chelators for ^{89}Zr -Labeling of Biomolecules: Investigation of Chemical/Radiochemical Properties and Complex Stability. <i>Cancers</i> , 2021, 13, 6349. | 1.7 | 12 |
| 16286 | Methylation with Dimethyl Carbonate/Dimethyl Sulfide Mixtures: An Integrated Process without Addition of Acid/Base and Formation of Residual Salts. <i>ChemSusChem</i> , 2022, 15, e202102538. | 3.6 | 8 |
| 16287 | Radical Perfluoroalkylation Enabled by a Catalytically Generated Halogen Bonding Complex and Visible Light Irradiation. <i>Organic Letters</i> , 2022, 24, 446-450. | 2.4 | 27 |
| 16288 | The 6.2 μm PAH Feature and the Role of Nitrogen: Revisited. <i>Astrophysical Journal</i> , 2021, 923, 202. | 1.6 | 11 |
| 16289 | Drug Discovery for Mycobacterium tuberculosis Using Structure-Based Computer-Aided Drug Design Approach. <i>International Journal of Molecular Sciences</i> , 2021, 22, 13259. | 1.8 | 30 |
| 16290 | DFT study on the gold(I)-catalyzed cycloaddition and rearrangement reactions of allene-containing allylic silyl ether. <i>Journal of Molecular Modeling</i> , 2022, 28, 25. | 0.8 | 2 |
| 16291 | Binding Energy and Free Energy of Calcium Ion to Calmodulin EF-Hands with the Drude Polarizable Force Field. <i>ACS Physical Chemistry Au</i> , 2022, 2, 143-155. | 1.9 | 7 |
| 16292 | Iridium(VII) "Corrole Terminal Carbides Should Exist as Stable Compounds. <i>ACS Organic & Inorganic Au</i> , 2022, 2, 159-163. | 1.9 | 4 |
| 16293 | Study of the Electronic Structure of $\text{M}_2(\text{CH}_2)_2(\text{CMe}_3)_6$ (M = Mo, W) by Photoelectron Spectroscopy and Density Functional Theory. <i>Organometallics</i> , 2022, 41, 29-40. | 1.1 | 1 |
| 16294 | Large-Scale Screening Reveals That Geometric Structure Matters More Than Electronic Structure in the Bioinspired Catalyst Design of Formate Dehydrogenase Mimics. <i>ACS Catalysis</i> , 2022, 12, 383-396. | 5.5 | 5 |
| 16295 | Ambimodal Pericyclic Rearrangements of Dialkenyl-Bullvalenes Give Tetrahydro-1,8-ethenoheptalenes. <i>Organic Letters</i> , 2022, 24, 319-323. | 2.4 | 2 |
| 16296 | Benchmarking the Accuracy of the Direct Random Phase Approximation and f -Functionals for NMR Shieldings. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 192-205. | 2.3 | 3 |
| 16297 | Taking Advantage of a Systematic Energy Non-linearity Error in Density Functional Theory for the Calculation of Electronic Energy Levels. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10507-10513. | 1.1 | 5 |
| 16298 | Quantum Mechanical Investigation on Decomposition Pathways of BuNENA. <i>Propellants, Explosives, Pyrotechnics</i> , 2022, 47, . | 1.0 | 0 |
| 16299 | Fungicidal amphotericin B sponges are assemblies of staggered asymmetric homodimers encasing large void volumes. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 972-981. | 3.6 | 10 |
| 16300 | Sono-Cavitation and Nebulization-Based Synthesis of Conjugated Microporous Polymers for Energy Storage Applications. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 61598-61609. | 4.0 | 19 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16301 | Accurate X-ray Absorption Spectra near L- and M-Edges from Relativistic Four-Component Damped Response Time-Dependent Density Functional Theory. <i>Inorganic Chemistry</i> , 2022, 61, 830-846. | 1.9 | 12 |
| 16302 | Modular and stereoselective synthesis of tetrasubstituted vinyl sulfides leading to a library of AIEgens. <i>Nature Communications</i> , 2021, 12, 7298. | 5.8 | 24 |
| 16303 | Nâ•N Bond Cleavage by Tantalum Hydride Complexes: Mechanistic Insights and Reactivity. <i>Inorganic Chemistry</i> , 2022, 61, 474-485. | 1.9 | 5 |
| 16304 | Synthesis, structural, spectroscopic and docking studies on (E)-1-Ferrocenyl-3-phenylâpropen-1-one by the density functional theory. <i>Molecular Simulation</i> , 2022, 48, 387-402. | 0.9 | 0 |
| 16305 | Computational Design of Rhenium(I) Carbonyl Complexes for Anticancer Photodynamic Therapy. <i>Inorganic Chemistry</i> , 2022, 61, 439-455. | 1.9 | 6 |
| 16306 | Towards low-energy-light-driven bistable photoswitches: ortho-fluoroaminoazobenzenes. <i>Photochemical and Photobiological Sciences</i> , 2022, 21, 159-173. | 1.6 | 15 |
| 16307 | Theoretical Investigation on the Rhodium-Catalyzed Annulation of 2-Phenyl-1H-indole with Ethyl 2-Diazo-3-oxo-3-phenylpropanoate. <i>Russian Journal of Physical Chemistry A</i> , 2021, 95, 2573-2577. | 0.1 | 0 |
| 16308 | ð•Ñ, ðµð°Ñ, ð²ð½Ñ – ð°Ñ, ð¾ð¼ð½Ñ – ð•ð°Ñ€Ñð, ð°ð°ð½ð¾ð½Ñ – Ñ½ð½ð, Ñ... 2'•ðµð•ð¾ð°Ñ, Ñ€ð, ð¾ð¾ð½Ñfð°ð»ð | | |
| 16309 | Synthesis, antibacterial and antioxidant activities of Thiazole-based Schiff base derivatives: a combined experimental and computational study. <i>BMC Chemistry</i> , 2021, 15, 67. | 1.6 | 30 |
| 16310 | Extraction of a One-Particle Reduced Density Matrix from a Quantum Monte Carlo Electronic Density: A New Tool for Studying Nondynamic Correlation. <i>Computation</i> , 2021, 9, 135. | 1.0 | 1 |
| 16311 | Ab Initio Molecular Dynamics Assessment on the Mixed Ionicâ€Electronic Transport for Crystalline Poly(3-Hexylthiophene) Using Full Explicit Lithium-Based Dopants and Additives. <i>Macromolecules</i> , 2022, 55, 113-124. | 2.2 | 6 |
| 16312 | Tandem Michaelâ€anti</i>-Michael Addition-Mediated Orthogonal Strapping of Dinyones: Regioselective Spirocyclopentannulation of Oxindoles and Pyrazolones and DFT Validation. <i>Journal of Organic Chemistry</i> , 2022, 87, 884-891. | 1.7 | 14 |
| 16313 | Why Does a B₁₂H₁₂ Icosahedron Need Two Electrons to be Stable: A First-Principles Electron-Correlated Investigation of B₁₂H_n (<i>n</i> =) Tj ETQq0 0.0 rgBT /Qverlock 10 | | |
| 16314 | Elucidation of kinetic and structural properties of eye lens Îƒ-crystallin: an <i>in vitro</i> and <i>in silico</i> approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 1178-1192. | 2.0 | 18 |
| 16315 | Hydrogen Delocalization in an Asymmetric Biomolecule: The Curious Case of Alpha-Fenchol. <i>Molecules</i> , 2022, 27, 101. | 1.7 | 1 |
| 16316 | Combined Spectroscopic and Computational Investigation on the Oxidation of <i>exo</i>-Tetrahydrodicyclopentadiene (JP-10; C₁₀H₁₆) Doped with Titaniumâ€Aluminumâ€Boron Reactive Metal Nanopowder. <i>Journal of Physical Chemistry A</i> , 2022, 126, 125-144. | 1.1 | 10 |
| 16317 | Composition Related Tunability of â€Greenâ€Core/Shell Quantum Dots for Photovoltaic Applications from First Principles. <i>Journal of Physical Chemistry C</i> , 2021, 125, 27046-27057. | 1.5 | 8 |
| 16318 | Synthesis and characterization of rhenia[10]annulynes. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 2895-2902. | 3.0 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16319 | Structure, Bonding and Adaptive Aromaticity in Rhenium-oxo Complexes: A DFT Study. <i>New Journal of Chemistry</i> , 0, , . | 1.4 | 5 |
| 16320 | Theoretical unraveling of the separation of trivalent Am and Eu ions by phosphine oxide ligands with different central heterocyclic moieties. <i>Dalton Transactions</i> , 2022, 51, 7118-7126. | 1.6 | 10 |
| 16321 | A DFT study of NHC-catalyzed reactions between 2-bromo-2-enals and acylhydrazones: mechanisms, and chemo- and stereoselectivities. <i>New Journal of Chemistry</i> , 2022, 46, 9146-9154. | 1.4 | 3 |
| 16322 | Isolation of the elusive bisbenzimidazole Bbim ³⁺ radical anion and its employment in a metal complex. <i>Chemical Science</i> , 2022, 13, 5818-5829. | 3.7 | 6 |
| 16323 | Probing computational methodologies in predicting mid-infrared spectra for large polycyclic aromatic hydrocarbons. <i>Monthly Notices of the Royal Astronomical Society</i> , 2022, 513, 3663-3681. | 1.6 | 9 |
| 16324 | The critical role of Asp206 stabilizing residues on the catalytic mechanism of the <i>Ideonella sakaiensis</i> PETase. <i>Catalysis Science and Technology</i> , 2022, 12, 3474-3483. | 2.1 | 4 |
| 16325 | An energetics assessment of benzo[<i>a</i>]tetracene and benzo[<i>a</i>]pyrene as triplet-triplet annihilation emitters. <i>Molecular Systems Design and Engineering</i> , 2022, 7, 889-898. | 1.7 | 2 |
| 16326 | Highly-fluorescent BODIPY-functionalised metallocages as drug delivery systems: synthesis, characterisation and cellular accumulation studies. <i>Dalton Transactions</i> , 2022, 51, 7476-7490. | 1.6 | 8 |
| 16327 | Synthesis, Structure, and Spectral Properties of Perhalogenated Metalloporphyrins. <i>Russian Journal of Inorganic Chemistry</i> , 2022, 67, 267-275. | 0.3 | 2 |
| 16328 | Atomistic modeling of Li- and post-Li-ion batteries. <i>Physical Review Materials</i> , 2022, 6, . | 0.9 | 17 |
| 16329 | Elastic and phonon-mode anomalies with temperature in the energetic material $C_6H_6N_4O_8$. <i>Journal of Chemical Physics</i> , 2022, 156, 154114. | 1.1 | 1 |
| 16330 | Origin invariant electronic circular dichroism in the length dipole gauge without London atomic orbitals. <i>Journal of Chemical Physics</i> , 2022, 156, 154114. | 1.2 | 7 |
| 16331 | Conformation-related excited-state charge transfer/separation of donor-acceptor chromophores. <i>Journal of Chemical Physics</i> , 2022, 156, 174902. | 1.2 | 4 |
| 16332 | Anion-Containing Solvation Structure Reconfiguration Enables Wide-Temperature Electrolyte for High-Energy-Density Lithium-Metal Batteries. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 19056-19066. | 4.0 | 18 |
| 16333 | Relativistic Orbital-Optimized Density Functional Theory for Accurate Core-Level Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3438-3449. | 2.1 | 24 |
| 16334 | Quinoline-fused both non-peripheral and peripheral Zn ^{II} and Mg ^{II} phthalocyanines: Anti-cholinesterase, anti-glucosidase, DNA nuclease, antioxidant activities, and in silico studies. <i>Applied Organometallic Chemistry</i> , 2022, 36, . | 1.7 | 10 |
| 16335 | Silyl-Functionalized Electrolyte Additives and Their Reactivity toward Lewis Bases in Li-Ion Cells. <i>Chemistry of Materials</i> , 2022, 34, 3831-3838. | 3.2 | 6 |
| 16336 | Penta-belt: A new carbon nanobelt. <i>Journal of Molecular Structure</i> , 2022, 1263, 133055. | 1.8 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16337 | Pro-Dipeptide Thiourea Organocatalyst in the Mannich Reaction between α -Amino Esters and Pyruvates. <i>European Journal of Organic Chemistry</i> , 2022, 2022, . | 1.2 | 2 |
| 16338 | B ₆ C ₈ and its anion: a planar dodecagon reinforced by the central strong B-B single bond and aromaticity. <i>Theoretical Chemistry Accounts</i> , 2022, 141, 1. | 0.5 | 1 |
| 16339 | From Molecules with a Planar Tetracoordinate Carbon to an Astronomically Known C ₅ H ₂ Carbene. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2561-2568. | 1.1 | 14 |
| 16340 | Structures, Energetics, and Spectra of (NH) and (OH) Tautomers of 2-(2-Hydroxyphenyl)-1-azaazulene: A Density Functional Theory/Time-Dependent Density Functional Theory Study. <i>ACS Omega</i> , 2022, 7, 14222-14238. | 1.6 | 4 |
| 16341 | Computational study on the mechanism of metal-free photochemical borylation of aryl halides. <i>International Journal of Quantum Chemistry</i> , 2022, 122, . | 1.0 | 3 |
| 16342 | 3-Input AND Molecular Logic Gate with Enhanced Fluorescence Output: The Key Atom for the Accurate Prediction of the Spectra. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 6436-6448. | 2.5 | 5 |
| 16343 | Three-State Switching of an Fe Spin Crossover Complex. <i>Journal of Physical Chemistry C</i> , 2022, 126, 7238-7244. | 1.5 | 2 |
| 16344 | Improving Discharge Voltage of Al-Air Batteries by Ga ³⁺ Additives in NaCl-Based Electrolyte. <i>Nanomaterials</i> , 2022, 12, 1336. | 1.9 | 8 |
| 16345 | Mechanism and Origins of Enantioselectivity of Cobalt-Catalyzed Intermolecular Hydroarylation/Cyclization of 1,6-Enynes with <i>i</i> -N-Pyridylindoles. <i>Journal of Organic Chemistry</i> , 2022, 87, 6438-6443. | 1.7 | 15 |
| 16346 | Hyperbranched phthalocyanine enabling black-phase formamidinium perovskite solar cells processing and operating in humidity open air. <i>Journal of Energy Chemistry</i> , 2022, 71, 141-149. | 7.1 | 10 |
| 16347 | Cp ₂ TiCl ₂ : Synthesis, Characterization, Modeling and Catalysis. <i>Journal of Chemical Education</i> , 2022, 99, 2121-2128. | 1.1 | 5 |
| 16348 | Synthesis and Investigation of Novel CHCA-Derived Matrices for Matrix-Assisted Laser Desorption/Ionization Mass Spectrometric Analysis of Lipids. <i>Molecules</i> , 2022, 27, 2565. | 1.7 | 4 |
| 16349 | Examining the Role of Aryldiazonium Salts in Surface Electroinitiated Polymerization. <i>Langmuir</i> , 2022, 38, 4979-4995. | 1.6 | 5 |
| 16350 | Water Network Shape-Dependence of Local Interactions with the Microhydrated NO_2^+ and CO_2^+ Anionic Head Groups by Cold Ion Vibrational Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2471-2479. | 1.1 | 2 |
| 16351 | Protonated Chiral 1,2-Diamine Organocatalysts for N-Selective Nitroso Aldol Reaction. <i>Catalysts</i> , 2022, 12, 435. | 1.6 | 1 |
| 16352 | A ratiometric fluorescent sensor based azo compound of 4-(4-Dimethylamino-phenylazo)-N-pyridin-2-ylmethyl-benzamide for rapid and selective detection of Fe ³⁺ ion. <i>Journal of Molecular Liquids</i> , 2022, 358, 119168. | 2.3 | 5 |
| 16353 | Insight into the relationship between molecular morphology and water/ion diffusion in cation exchange membranes: Case of partially sulfonated polyether sulfone. <i>Journal of Membrane Science</i> , 2022, 654, 120561. | 4.1 | 7 |
| 16354 | Optoelectronic properties by solution technique and comprehensive solvatochromism of novel fluorescent Schiff base derivatives. <i>Journal of Molecular Liquids</i> , 2022, 357, 119110. | 2.3 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16355 | Controlled C–H bond activation leads to orthometalation and ring-hydroxylation in Ni(II) and Pd(II) complexes of a common tridentate azophenyl-salicylaldehyde ligand. <i>Inorganica Chimica Acta</i> , 2022, 538, 120960. | 1.2 | 1 |
| 16382 | A theoretical investigation into gallic acid pyrolysis. <i>Journal of Computational Chemistry</i> , 2022, 43, 1023-1032. | 1.5 | 5 |
| 16383 | Identification of potential andrographolide-based drug candidate against Keap1-Nrf2 pathway through rigorous cheminformatics screening. <i>Molecular Diversity</i> , 2022, , 1. | 2.1 | 0 |
| 16384 | An Aluminum-Based Metal-Organic Cage for Cesium Capture. <i>Inorganic Chemistry</i> , 2022, 61, 6604-6611. | 1.9 | 7 |
| 16385 | Evaluating the Effects of Metal Adduction and Charge Isomerism on Ion-Mobility Measurements using <i>m</i> -Xylene Macrocycles as Models. <i>Journal of the American Society for Mass Spectrometry</i> , 2022, 33, 840-850. | 1.2 | 8 |
| 16386 | Nature-derived epoxy resins: Synthesis, allergenicity, and thermosetting properties of pinosresinol diglycidyl ether. <i>Toxicology and Industrial Health</i> , 2022, 38, 259-269. | 0.6 | 7 |
| 16387 | Calculated linear and nonlinear optical absorption spectra of phosphine-ligated gold clusters. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11234-11248. | 1.3 | 1 |
| 16388 | Various bond interactions between NO and anionic gold clusters: a theoretical calculation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 13641-13650. | 1.3 | 1 |
| 16389 | Water on porous, nitrogen-containing layered carbon materials: the performance of computational model chemistries. <i>Physical Chemistry Chemical Physics</i> , 2022, , . | 1.3 | 0 |
| 16390 | A straightforward method to quantify the electron-delocalizing ability of π -conjugated molecules. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11486-11490. | 1.3 | 3 |
| 16391 | Selection Mechanism of Synergistic Effect between Dielectric Barrier Discharge Plasma and Cu ^{II} -Al ₂ O ₃ Catalyst in Carbonyl-Sulfide Conversion: Electric Field Changes Energy Barrier and Reaction Path. <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 0 |
| 16392 | Why Local and Non-local Terms are Essential for Second Harmonic Generation Simulation?. <i>Physical Chemistry Chemical Physics</i> , 2022, , . | 1.3 | 3 |
| 16393 | Synthesis, characterization and application of oxovanadium(<i>iv</i>) complexes with [NNO] donor ligands: X-ray structures of their corresponding dioxovanadium(<i>v</i>) complexes. <i>RSC Advances</i> , 2022, 12, 13740-13748. | 1.7 | 3 |
| 16394 | A conjugated photoresponsive dithienylethene-ferrocene system: applications in secret writing and decoding information. <i>Journal of Materials Chemistry C</i> , 2022, 10, 8860-8873. | 2.7 | 5 |
| 16395 | Charge transfer in mixed and segregated stacks of tetrathiafulvalene, tetrathianaphthalene and naphthalene diimide: a structural, spectroscopic and computational study. <i>New Journal of Chemistry</i> , 0, , . | 1.4 | 0 |
| 16396 | Ultrasensitive and Rapid Colorimetric Detection of Urotropin Boosted by Effective Electrostatic Probing and Non-Covalent Sampling. <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 0 |
| 16397 | Noncovalently bound excited-state dimers: a perspective on current time-dependent density functional theory approaches applied to aromatic excimer models. <i>RSC Advances</i> , 2022, 12, 13014-13034. | 1.7 | 18 |
| 16398 | Composition-driven archetype dynamics in polyoxovanadates. <i>Chemical Science</i> , 2022, 13, 6397-6412. | 3.7 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16399 | TAO-DFT fictitious temperature made simple. RSC Advances, 2022, 12, 12193-12210. | 1.7 | 7 |
| 16400 | Investigating the competing E2 and S _N 2 mechanisms for the microsolvated HO ⁺ (H ₂ O) _n + CH ₃ CH ₂ X (X =) TjEQ1108784314 | 1.3 | 1 |
| 16401 | Customising excitation properties of polycyclic aromatic hydrocarbons by rational positional heteroatom doping: the peri-xanthenoxanthene (PXX) case. Chemical Science, 0, , . | 3.7 | 5 |
| 16402 | A phosphonic acid anion and acid dimer dianion stabilized by proton transfer in OHN hydrogen bonds models of structural motifs in blend polymer membranes. Physical Chemistry Chemical Physics, 2022, 24, 11362-11369. | 1.3 | 1 |
| 16403 | Relativistic DFT Calculations of Changes in NMR Chemical Shifts in Aqueous Solutions of Heavy-Metal Nitrates. Journal of Computer Chemistry Japan -International Edition, 2022, 8, n/a. | 0.2 | 0 |
| 16404 | Efficient Charge Transport Driven by Strong Intermolecular Interactions in Cyclopentadithiophene-Based Donor-Acceptor Type Conjugated Copolymers. Advanced Electronic Materials, 2022, 8, . | 2.6 | 8 |
| 16405 | The influence of a solvent environment on direct non-covalent interactions between two molecules: A symmetry-adapted perturbation theory study of polarization tuning of interactions by water. Journal of Chemical Physics, 2022, 156, . | 1.2 | 6 |
| 16406 | Direct Electron Transfer between Aromatic Molecules inside and outside the ZSM-5 Zeolite Channels: An Identification of the EPR Spectra of 1,3,5-Trimethylbenzene Radical Cations. Journal of Physical Chemistry C, 2022, 126, 7421-7430. | 1.5 | 0 |
| 16407 | Organic-Inorganic Composite Electrolytes Optimized with Fluoroethylene Carbonate Additive for Quasi-Solid-State Lithium-Metal Batteries. ACS Applied Materials & Interfaces, 2022, 14, 20962-20971. | 4.0 | 19 |
| 16408 | pH-Controlled Intramolecular Decarboxylative Cyclization of Biarylacetic Acids: Implication on Umpolung Reactivity of Aroyl Radicals. Journal of Organic Chemistry, 2022, 87, 6638-6656. | 1.7 | 4 |
| 16409 | Structure, IR and Raman spectra of the optically active quaternized ammonium salt promising object for liquid crystal systems. Molecular Crystals and Liquid Crystals, 0, , 1-9. | 0.4 | 0 |
| 16410 | Differences in the Structure and Antimicrobial Activity of Hydrazones Derived from Methyl 4-Phenylpicolinimidate. Materials, 2022, 15, 3085. | 1.3 | 3 |
| 16411 | Enantioselective Organocatalyzed Michael Addition of Isobutyraldehyde to Maleimides in Aqueous Media. Molecules, 2022, 27, 2759. | 1.7 | 0 |
| 16412 | Study the transition state of SnO ₂ cluster with NO ₂ gas molecule via density functional theory. International Journal of Nanoscience, 0, , . | 0.4 | 0 |
| 16413 | Binding and Degradation Reaction of Hydroxide Ions with Several Quaternary Ammonium Head Groups of Anion Exchange Membranes Investigated by the DFT Method. Molecules, 2022, 27, 2686. | 1.7 | 12 |
| 16414 | New Strategies for Direct Methane-to-Methanol Conversion from Active Learning Exploration of 16 Million Catalysts. JACS, 2022, 144, 1200-1213. | 3.6 | 23 |
| 16415 | Molecular Modeling of Biofuel Cells of BN Nanotube-FAD Structure. Russian Journal of Physical Chemistry A, 2022, 96, S105-S112. | 0.1 | 1 |
| 16416 | Unlocking New Redox Activity in Alluaudite Cathodes through Compositional Design. Chemistry of Materials, 2022, 34, 4088-4103. | 3.2 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16417 | Phosphine Ligand Binding and Catalytic Activity of Group 10 ¹⁴ Heterobimetallic Complexes. <i>Inorganic Chemistry</i> , 2022, 61, 6888-6897. | 1.9 | 1 |
| 16418 | Investigation of water substitution at $\langle \text{sc} \rangle \text{Ru} \langle \text{sup} \rangle \text{II} \langle \text{sup} \rangle \langle \text{sc} \rangle$ complexes by conceptual $\langle \text{sc} \rangle$ density function theory $\langle \text{sc} \rangle$ approach. <i>Journal of Computational Chemistry</i> , 2022, 43, 1161-1175. | 1.5 | 2 |
| 16419 | Chiral effect on A β 2 fibrillation from molecular-scale to nanoscale. <i>Nano Research</i> , 2022, 15, 6721-6729. | 5.8 | 6 |
| 16420 | Theoretical Insights on the Two-Dimensional Transitional Metal Trihydroxytriaminophenalenyl for Highly Efficient Carbon Dioxide Electroreduction. <i>Journal of the Electrochemical Society</i> , 2022, 169, 056512. | 1.3 | 0 |
| 16421 | Cosolvent Simulations with Fragment-Bound Proteins Identify Hot Spots to Direct Lead Growth. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3829-3844. | 2.3 | 4 |
| 16422 | Ultra-high-rate lithium-sulfur batteries with high sulfur loading enabled by Mn2O3-carbonized bacterial cellulose composite as a cathode host. <i>Electrochimica Acta</i> , 2022, 422, 140531. | 2.6 | 24 |
| 16423 | LFDFT ² A Practical Tool for Coordination Chemistry. <i>Computation</i> , 2022, 10, 70. | 1.0 | 3 |
| 16424 | Prediction of COMT Inhibitors Using Machine Learning and Molecular Dynamics Methods. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3477-3492. | 1.2 | 2 |
| 16425 | Vibrational spectroscopy studies of methacrylic polymers containing heterocyclic azo dyes. <i>Vibrational Spectroscopy</i> , 2022, 120, 103377. | 1.2 | 2 |
| 16426 | Revisiting the Performance of Time-Dependent Density Functional Theory for Electronic Excitations: Assessment of 43 Popular and Recently Developed Functionals from Rungs One to Four. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3460-3473. | 2.3 | 61 |
| 16427 | Effect of support hydrophobicity of halloysite α -based catalysts on the polyalphaolefin hydrofinishing performance. <i>Applied Organometallic Chemistry</i> , 2022, 36, . | 1.7 | 16 |
| 16428 | Refined Data on the Sublimation Enthalpy and Thermodynamic Functions of $\langle \text{sc} \rangle \text{I} \langle \text{sc} \rangle$ - and $\langle \text{sc} \rangle \text{dl} \langle \text{sc} \rangle$ -Methionine. <i>Journal of Chemical & Engineering Data</i> , 2022, 67, 1326-1334. | 1.0 | 2 |
| 16429 | Three-Dimensional Fully π -Conjugated Macrocycles: When 3D-Aromatic and When 2D-Aromatic-in-3D?. <i>Journal of the American Chemical Society</i> , 2022, 144, 8560-8575. | 6.6 | 28 |
| 16430 | Efficient removal of organophosphate esters by ligand functionalized MIL-101 (Fe): Modulated adsorption and DFT calculations. <i>Chemosphere</i> , 2022, 302, 134881. | 4.2 | 21 |
| 16431 | When Identification of the Reduction Sites in Mixed Molybdenum/Tungsten Keggin-Type Polyoxometalate Hybrids Turns Out Tricky. <i>Inorganic Chemistry</i> , 2022, 61, 7700-7709. | 1.9 | 3 |
| 16432 | Transition orbital projection approach for excited state tracking. <i>Journal of Chemical Physics</i> , 2022, 156, . | 1.2 | 2 |
| 16433 | Gas-Phase Reactivity of Phenylcarbyne Anions. <i>Journal of the American Chemical Society</i> , 2022, 144, 8576-8590. | 6.6 | 10 |
| 16434 | Thiazole Containing PNA Mimic Regulates <i>c-MYC</i> Gene Expression through DNA G-Quadruplex. <i>Bioconjugate Chemistry</i> , 2022, 33, 1145-1155. | 1.8 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 16435 | Testing the limitations of harmonic approximation in the determination of Raman intensities. <i>Molecular Physics</i> , 2022, 120, . | 0.8 | 1 |
| 16436 | Volatile Products of the Autoxidation of Poly(ethylenimine) in CO ₂ Sorbents. <i>Journal of Physical Chemistry C</i> , 2022, 126, 8807-8816. | 1.5 | 9 |
| 16437 | A Low-Potential and Stable Bis-Dimethylamino Substituted Anthraquinone for pH-Neutral Aqueous Redox Flow Batteries. <i>ChemElectroChem</i> , 0, . | 1.7 | 4 |
| 16438 | Hydrogen Bond-Assisted Fluoride Binding by a Stiborane. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2022, 648, . | 0.6 | 1 |
| 16439 | Conformational Landscape of the Hydrogen-Bonded 1-Phenyl-2,2,2-Trifluoroethanol-1,4-Dioxane Complex: Dispersion Interactions and Conformational Conversion. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2942-2949. | 1.1 | 4 |
| 16440 | Template Synthesis of NPN ²⁻ Pincer-type Ligands at Titanium Using an Ambiphilic Phosphide Scaffold. <i>Inorganic Chemistry</i> , 2022, 61, 7642-7653. | 1.9 | 2 |
| 16441 | HCnH ⁻ Anion Chains with n ≥ 8 Are Nonlinear and Their Permanent Dipole Makes Them Potential Candidates for Astronomical Observation. <i>Molecules</i> , 2022, 27, 3100. | 1.7 | 7 |
| 16442 | Energy Decomposition Analysis of the Nature of Coordination Bonding at the Heme Iron Center in Cytochrome P450 Inhibition. <i>Chemistry - an Asian Journal</i> , 2022, 17, . | 1.7 | 4 |
| 16443 | Simple Rules for Complex Near-Glass-Transition Phenomena in Medium-Sized Schiff Bases. <i>International Journal of Molecular Sciences</i> , 2022, 23, 5185. | 1.8 | 3 |
| 16444 | Improving the Accuracy of Atomistic Simulations of the Electrochemical Interface. <i>Chemical Reviews</i> , 2022, 122, 10651-10674. | 23.0 | 39 |
| 16445 | New Insights into the Recognition and Sensing Mechanism of a H ₂ S Fluorescent Probe: A Theoretical Perspective. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2788-2793. | 1.1 | 2 |
| 16446 | Increasing Complexity in a Conformer Space Step-by-Step: Weighing London Dispersion against Cation-π Interactions. <i>Journal of the American Chemical Society</i> , 2022, 144, 9007-9022. | 6.6 | 13 |
| 16447 | NHC Catalyzed α -Carbon functionalization of carboxylic esters towards formation of α -Lactams: A mechanistic study. <i>Molecular Catalysis</i> , 2022, 524, 112311. | 1.0 | 0 |
| 16448 | Discovery of cinnamamide-barbiturate hybrids as a novel class of Nrf2 activator against myocardial ischemia/reperfusion injury. <i>Bioorganic Chemistry</i> , 2022, 124, 105828. | 2.0 | 2 |
| 16449 | Carbonate-free CoAl layered double hydroxides supercapacitors: Controlled precipitation via acid mediated decomplexation. <i>Applied Clay Science</i> , 2022, 224, 106519. | 2.6 | 5 |
| 16450 | Mechanism study of Cd(II) ion adsorption onto resins with sulfonic/phosphonic groups using electronic structure methods. <i>Journal of Molecular Liquids</i> , 2022, 358, 119199. | 2.3 | 6 |
| 16451 | Theoretical investigation of the electronic structure of the ground and lowest excited states with dipole moment and rovibrational calculations of the CuSe molecule. <i>Chemical Physics Letters</i> , 2022, 800, 139653. | 1.2 | 0 |
| 16452 | Flavanols from <i>Tetrapleura tetraptera</i> with cytotoxic activities. <i>FIToterap</i> , 2022, 160, 105206. | 1.1 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 16453 | Understanding of benzimidazole based ionic liquid as an efficient corrosion inhibitor for carbon steel: Experimental and theoretical studies. <i>Journal of Molecular Liquids</i> , 2022, 358, 119204. | 2.3 | 9 |
| 16454 | Resorcin[4]arene-based [Co12] supermolecule cage functionalized by bio-inspired [Co4O4] cubanes for visible light-driven water oxidation. <i>Inorganic Chemistry Communication</i> , 2022, 141, 109514. | 1.8 | 1 |
| 16455 | Constructing high-accuracy theoretical Raman spectra of SARS-CoV-2 spike proteins based on a large fragment method. <i>Chemical Physics Letters</i> , 2022, 800, 139663. | 1.2 | 4 |
| 16456 | In-depth insight into the mechanism on photocatalytic synergistic removal of antibiotics and Cr (VI): The decisive effect of antibiotic molecular structure. <i>Applied Catalysis B: Environmental</i> , 2022, 313, 121443. | 10.8 | 60 |
| 16457 | Photophysical characteristics of Phenylimidazo(4,5-f)1,10-phenanthroline Rhenium(II) complexes - A theoretical approach to their potential applications in lighting devices. <i>Materials Science in Semiconductor Processing</i> , 2022, 147, 106733. | 1.9 | 0 |
| 16458 | Characteristics of nitrogen oxide emissions from combustion synthesis of a CuO oxygen carrier. <i>Fuel Processing Technology</i> , 2022, 233, 107295. | 3.7 | 7 |
| 16459 | Computational redox chemistry of functionalized Polycaprolactone as electrolytes for lithium batteries. <i>Journal of Electroanalytical Chemistry</i> , 2022, 916, 116377. | 1.9 | 2 |
| 16460 | Spectroscopic investigation of the electronic and excited state properties of para-substituted tetraphenyl porphyrins and their electrochemically generated ions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 278, 121300. | 2.0 | 6 |
| 16461 | Synthesis, experimental antimicrobial activity, theoretical vibrational analysis, quantum chemical modeling and molecular docking studies of (E)-4-(benzylideneamino)benzenesulfonamide. <i>Journal of Molecular Structure</i> , 2022, 1263, 133187. | 1.8 | 38 |
| 16462 | Thermally activated delayed fluorescence poly(dendrimer)s " detrapping excitons for reverse intersystem crossing. <i>Journal of Materials Chemistry C</i> , 2022, 10, 8109-8124. | 2.7 | 1 |
| 16463 | Transition metal complexes of the PPO/POP ligand: variable coordination chemistry and photo-luminescence properties. <i>Dalton Transactions</i> , 2022, 51, 8975-8985. | 1.6 | 2 |
| 16464 | Highly regioselective tandem hydroformylation of substituted styrene using Iminophosphine rhodium complex immobilized on carbon. <i>Journal of Industrial and Engineering Chemistry</i> , 2022, 112, 218-232. | 2.9 | 7 |
| 16465 | Real Temperature Model of Dynamic Disorder in Molecular Crystals. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3265-3272. | 1.1 | 3 |
| 16466 | Pd/NHC-Controlled Regiodivergent Defluorinative Allylation of gem-Difluorocyclopropanes with Allylboronates. <i>ACS Catalysis</i> , 2022, 12, 6495-6505. | 5.5 | 30 |
| 16467 | A New Benzoxazole-Based Fluorescent Macrocyclic Chemosensor for Optical Detection of Zn ²⁺ and Cd ²⁺ . <i>Chemosensors</i> , 2022, 10, 188. | 1.8 | 13 |
| 16468 | Conformational landscape and internal dynamics of limona ketone, a key oxidation product of limonene. <i>Journal of Molecular Spectroscopy</i> , 2022, 387, 111643. | 0.4 | 1 |
| 16469 | Difficulty of the evaluation of the barrier height of an open-shell transition state between closed shell minima: the case of small C _{4n} rings. <i>Journal of Chemical Physics</i> , 0, , . | 1.2 | 2 |
| 16470 | Recommendation of Orbitals for GW Calculations on Molecules and Crystals. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3523-3537. | 2.3 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16471 | D-band frontier: A new hydrogen evolution reaction activity descriptor of Pt single-atom catalysts. <i>Journal of Energy Chemistry</i> , 2022, 72, 203-209. | 7.1 | 16 |
| 16472 | Assessing Recent Time-Dependent Double-Hybrid Density Functionals on Doublet Doublet Excitations. <i>ACS Physical Chemistry Au</i> , 2022, 2, 407-416. | 1.9 | 3 |
| 16473 | Influence and Mechanism of Polar Solvents on the Retention Time of Short-Chain Fatty Acids in Gas Chromatography. <i>Separations</i> , 2022, 9, 124. | 1.1 | 3 |
| 16474 | Density-functional theory vs density-functional fits. <i>Journal of Chemical Physics</i> , 2022, 156, . | 1.2 | 19 |
| 16475 | Enabling Scalable Polymer Electrolyte with Synergetic Ion Conductive Channels via a Two Stage Rheology Tuning UV Polymerization Strategy. <i>Small</i> , 2022, 18, e2202013. | 5.2 | 9 |
| 16476 | Ruthenium-Catalyzed Dehydrogenative Functionalization of Alcohols to Pyrroles: A Comparison between Metal-Ligand Cooperative and Non-cooperative Approaches. <i>Journal of Organic Chemistry</i> , 2022, 87, 7106-7123. | 1.7 | 12 |
| 16477 | Catalytic Enantioselective Synthesis of β -Lactams with β -Quaternary Centers via Merging of C-C Activation and Sulfonyl Radical Migration. <i>Journal of the American Chemical Society</i> , 2022, 144, 9222-9228. | 6.6 | 16 |
| 16478 | Electron transport through a (terpyridine)ruthenium metallo-surfactant containing a redox-active aminocatechol derivative. <i>Dalton Transactions</i> , 2022, 51, 8425-8436. | 1.6 | 3 |
| 16479 | Crystalline salts of a diuretic drug torasemide with improved solubility and dissolution properties. <i>CrystEngComm</i> , 2022, 24, 4235-4250. | 1.3 | 2 |
| 16480 | Theoretical mechanistic insights into the polar hydrohalogenation of olefins. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 4976-4985. | 1.5 | 2 |
| 16481 | Generation of singlet oxygen catalyzed by the room-temperature-stable anthraquinone anion radical. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14165-14171. | 1.3 | 2 |
| 16482 | Effectiveness of Organic Compounds in Coal Flotation: A Quantum Chemical Approach. <i>Coke and Chemistry</i> , 2022, 65, 76-79. | 0.0 | 0 |
| 16483 | A Non-Bornian Approach to the Standard Gibbs Energy of Ion Transfer at the Oil Water Interface. <i>Review of Polarography</i> , 2022, 68, 3-14. | 0.0 | 0 |
| 16484 | Adsorption of Benzene-1,4-diol, 3-Methyl-1,2-cyclopentanedione and 2,6-Dimethoxyphenol on aluminium (1 1 1) plane using density functional theory calculations. <i>Chemical Physics</i> , 2022, 560, 111592. | 0.9 | 3 |
| 16485 | Conformational Energy Benchmark for Longer n-Alkane Chains. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3521-3535. | 1.1 | 16 |
| 16486 | Electrochromic and photovoltaic properties of benzothiadiazole-based donor-acceptor conjugated polymers with oligo(ethylene glycol) side chains. <i>Dyes and Pigments</i> , 2022, 204, 110432. | 2.0 | 14 |
| 16487 | The antioxidant capacity of myricetin. A molecular electrostatic potential analysis based on DFT calculations. <i>Chemical Physics Letters</i> , 2022, 801, 139708. | 1.2 | 15 |
| 16488 | Efficient and simultaneous capture of iodine and methyl iodide achieved by a covalent organic framework. <i>Nature Communications</i> , 2022, 13, . | 5.8 | 101 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16489 | Practical electronic ground- and excited-state calculation method for lanthanide complexes based on frozen core potential approximation to 4f electrons. <i>Journal of Mathematical Chemistry</i> , 0, , . | 0.7 | 1 |
| 16490 | Pyrazole and Indazole Semihemiporphyrine Complexes of Rhenium Tricarbonyl: A Structure/Properties Study. <i>European Journal of Inorganic Chemistry</i> , 0, , . | 1.0 | 0 |
| 16491 | Mechanistic Studies of Oxygen-Atom Transfer (OAT) in the Homogeneous Conversion of N ₂ O by Ru Pincer Complexes. <i>Inorganics</i> , 2022, 10, 69. | 1.2 | 5 |
| 16492 | Tribology at the atomic scale with density functional theory. <i>Electronic Structure</i> , 2022, 4, 023002. | 1.0 | 3 |
| 16493 | A computational inspection of the dissociation energy of mid-sized organic dimers. <i>Journal of Chemical Physics</i> , 2022, 156, . | 1.2 | 5 |
| 16494 | Impact of π -Conjugation Length on the Excited-State Dynamics of Star-Shaped Carbazole- π -Triazine Organic Chromophores. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3291-3300. | 1.1 | 2 |
| 16495 | A CGA-ONIOM-DFT framework for accurate and efficient determination of thermodynamics and Kinetics: Case study of cyclopentane reaction with hydroxyl radical. <i>Chemical Physics Letters</i> , 2022, 801, 139714. | 1.2 | 0 |
| 16496 | A quantum-chemistry and molecular-dynamics study of non-covalent interactions between tri-n-butyl phosphate and 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide. <i>Journal of Molecular Liquids</i> , 2022, 360, 119430. | 2.3 | 8 |
| 16497 | Highly Efficient Removal of Organic Contaminant with Wide Concentration Range by a Novel Self-Cleaning Hydrogel: Mechanism, Degradation Pathway and Dft Calculation. <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 0 |
| 16498 | Ni(η^5 -Cp) ₂ complexes of a new tetradentate NNâ€²Nâ€²â€²O picolinoyl-1,2-phenylenediamide-phenolate redox-active ligand at different redox levels. <i>Dalton Transactions</i> , 0, , . | 1.6 | 2 |
| 16499 | Enhanced Photovoltaic Performance of D- π -A Organic Sensitizers by Simple Fluorination of Acceptor Unit. <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 0 |
| 16500 | Pyrolysis of Carbonyl Sulfide (Cos). <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 0 |
| 16501 | Development of Nd (III)-Based Terahertz Absorbers Revealing Temperature Dependent Near-Infrared Luminescence. <i>International Journal of Molecular Sciences</i> , 2022, 23, 6051. | 1.8 | 5 |
| 16502 | Unsaturated Dinitriles Formation Routes in Extraterrestrial Environments: A Combined Experimental and Theoretical Investigation of the Reaction between Cyano Radicals and Cyanoethene (C ₂ H ₃ CN). <i>Journal of Physical Chemistry A</i> , 2022, 126, 3569-3582. | 1.1 | 13 |
| 16503 | Synthesis of dielectric polystyrene via one-step nitration reaction for large-scale energy storage. <i>Chemical Engineering Journal</i> , 2022, 446, 137281. | 6.6 | 38 |
| 16504 | On the remarkable nonlinear optical properties of natural tomato lycopene. <i>Scientific Reports</i> , 2022, 12, . | 1.6 | 13 |
| 16505 | Twisting Enabled Charge Transfer Excitons in Epitaxially Fused Quantum Dot Molecules. <i>Nano Letters</i> , 2022, 22, 4912-4918. | 4.5 | 6 |
| 16506 | A mechanistic view of the reaction between phosphine and fluorine atom: Insights into PH ₃ F isomers. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113769. | 1.1 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16507 | Singlet Spin State Drives [V]-Carbene To Catalyze Olefin Metathesis: A Computational Analysis. Organometallics, 2022, 41, 1295-1303. | 1.1 | 4 |
| 16508 | Spirooxazine-Based Dual-Sensing Probe for Colorimetric Detection of Cu ²⁺ and Fe ³⁺ and Its Application in Drinking Water and Rice Quality Monitoring. ACS Omega, 2022, 7, 18671-18680. | 1.6 | 12 |
| 16509 | Ladder-like Polymer Brushes Containing Conjugated Poly(Propylenedioxythiophene) Chains. International Journal of Molecular Sciences, 2022, 23, 5886. | 1.8 | 8 |
| 16510 | Serine and Cysteine Peptidases: So Similar, Yet Different. How the Active-Site Electrostatics Facilitates Different Reaction Mechanisms. Journal of Physical Chemistry B, 2022, 126, 4035-4048. | 1.2 | 9 |
| 16511 | Computer-Aided Rational Construction of Mediated Bioelectrocatalysis with Î€-Conjugated (Hetero)cyclic Molecules: Toward Promoted Distant Electron Tunneling and Improved Biosensing. Analytical Chemistry, 2022, 94, 8033-8040. | 3.2 | 5 |
| 16512 | Design, Cytotoxicity and Antiproliferative Activity of 4-Amino-5-methyl-thieno[2,3-d]pyrimidine-6-carboxylates against MFC-7 and MDA-MB-231 Breast Cancer Cell Lines. Molecules, 2022, 27, 3314. | 1.7 | 3 |
| 16513 | Assembly and Thermal-Induced Polymerization of Histidine on Fumed Silica Surfaces. ACS Earth and Space Chemistry, 2022, 6, 1552-1562. | 1.2 | 0 |
| 16514 | Chiral Separation of Stilbene Dimers Generated by Biotransformation for Absolute Configuration Determination and Antibacterial Evaluation. Frontiers in Chemistry, 2022, 10, . | 1.8 | 3 |
| 16515 | On Aromaticity of the Aromatic Î±-Amino Acids and Tuning of the NICS Indices to Find the Aromaticity Order. Journal of Physical Chemistry A, 0, , . | 1.1 | 5 |
| 16516 | Water-in-Salt Electrolyte-Based Extended Voltage Range, Safe, and Long-Cycle-Life Aqueous Calcium-Ion Cells. ACS Applied Materials & Interfaces, 2022, 14, 25501-25515. | 4.0 | 15 |
| 16517 | Regression Modeling for the Prediction of Hydrogen Atom Transfer Barriers in Cytochrome P450 from Semi-empirically Derived Descriptors. Chemistry Methods, 2022, 2, . | 1.8 | 2 |
| 16518 | Synthesis, structural and electrochemical properties of a new family of amino-acid-based coordination complexes. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 520-536. | 0.5 | 1 |
| 16519 | Near-Infrared Absorbing Molecule Based on Triphenylamine Radical Cation with Extended Homoaryl Î€-System. Colorants, 2022, 1, 226-235. | 0.9 | 3 |
| 16520 | The structural origin of the efficient photochromism in natural minerals. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, . | 3.3 | 8 |
| 16521 | Theoretical insights into the linear relationship between $\log(k_{\text{H}}/k_{\text{H}_2\text{O}})$ and $\log(k_{\text{H}}/k_{\text{H}_2\text{O}})$ values and vibrational frequencies. Chemical Physics Letters, 2022, 803, 139746. | 1.2 | 10 |
| 16522 | Does Reduction-Induced Isomerization of a Uranium(III) Aryl Complex Proceed via C-H Oxidative Addition and Reductive Elimination across the Uranium(II/IV) Redox Couple?. Inorganic Chemistry, 2022, 61, 8955-8965. | 1.9 | 7 |
| 16523 | The High-Effective Catalytic Degradation of Benzo[a]pyrene by Mn-Corrolazine Regulated by Oriented External Electric Field: Insight From DFT Study. Frontiers in Chemistry, 2022, 10, . | 1.8 | 2 |
| 16524 | Structural Versatility and Energy Difference of Salt-Free Water Complex NaCl(H ₂ O) ₂ Encoded in Cryogenic Photoelectron Spectroscopy. Journal of Physical Chemistry Letters, 0, , 4995-5000. | 2.1 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 16525 | Millimeter-Wave Spectroscopy of Methylfuran Isomers: Local vs. Global Treatments of the Internal Rotation. <i>Molecules</i> , 2022, 27, 3591. | 1.7 | 1 |
| 16526 | Highly Selective Adsorption of Perfluorinated Greenhouse Gases by Porous Organic Cages. <i>Advanced Materials</i> , 2022, 34, . | 11.1 | 33 |
| 16527 | Biphasic Behaviors of Nd ³⁺ Bound with Cyanex272, Cyanex301, and Cyanex302: A Molecular Dynamics Simulation Study. <i>Inorganic Chemistry</i> , 2022, 61, 8920-8929. | 1.9 | 0 |
| 16528 | Enhanced steric effect and desolvation process on organic solvent nanofiltration: A mechanism study for removing anionic dyes. <i>Chemical Engineering Journal</i> , 2022, 446, 137360. | 6.6 | 4 |
| 16529 | Parallel arrangement of peptides appended to a rigid, bimetallic, constrained ring system. <i>Peptide Science</i> , 0, , . | 1.0 | 0 |
| 16530 | Assessment of perfluorohexane sulfonic acid (PFHxS)-related compounds degradation potential: Computational and experimental approaches. <i>Journal of Hazardous Materials</i> , 2022, 436, 129240. | 6.5 | 7 |
| 16531 | Study to amino acid-based inhibitors as an effective anti-corrosion material. <i>Journal of Molecular Liquids</i> , 2022, 360, 119449. | 2.3 | 7 |
| 16532 | Conformational and solvent effects in structural and spectroscopic properties of 2-hydroxyethyl methacrylate and acrylic acid. <i>Journal of Molecular Liquids</i> , 2022, 360, 119428. | 2.3 | 1 |
| 16533 | Synthesis, photophysical properties and two-photon absorption of benzothiazole/benzoxazole π -expanded carbazole dyes. <i>Dyes and Pigments</i> , 2022, 204, 110447. | 2.0 | 3 |
| 16534 | Ultrasensitive and rapid colorimetric detection of urotropin boosted by effective electrostatic probing and non-covalent sampling. <i>Journal of Hazardous Materials</i> , 2022, 436, 129263. | 6.5 | 6 |
| 16535 | Production of high-yield 5-hydroxymethylfurfural from crystalline cellulose via one-pot conversion in molten salt hydrate/acetone and separation. <i>Fuel</i> , 2022, 324, 124678. | 3.4 | 12 |
| 16536 | Synthesis, crystal structures, DFT calculations, and catalytic application in hydrosilylation of acetophenone derivatives with triethylsilane of novel rhodium-N-heterocyclic carbene (NHCs) complex. <i>Journal of Molecular Structure</i> , 2022, 1265, 133397. | 1.8 | 6 |
| 16539 | <i>Ab initio</i> derivation of flavin hyperfine interactions for the protein magnetosensor cryptochrome. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 16784-16798. | 1.3 | 4 |
| 16540 | Design of potential singlet fission chromophores based on diketofurofuran: an alternative to diketopyrrolopyrrole. <i>Journal of Materials Chemistry C</i> , 2022, 10, 10404-10411. | 2.7 | 3 |
| 16541 | Enhanced luminescence in multivariate metal-organic frameworks through an isolated-ligand strategy. <i>Journal of Materials Chemistry C</i> , 2022, 10, 10473-10479. | 2.7 | 7 |
| 16542 | Simulating the solvation structure of low- and high-spin [Fe(bpy) ₃] ²⁺ : long-range dispersion and many-body effects. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 16655-16670. | 1.3 | 3 |
| 16543 | Nitrene-Mediated Multicomponent Couplings and Macrocyclization by CH-Functionalization. <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 0 |
| 16544 | Theoretical Study of The Role of the Non-innocent Phenolate Ligand of a Nickel Complex in Water Oxidation. <i>Physical Chemistry Chemical Physics</i> , 0, , . | 1.3 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16545 | Unsaturated amido-substituted six-vertex mixed silicon germanium clusters. Dalton Transactions, 2022, 51, 10535-10542. | 1.6 | 2 |
| 16546 | A predictive chemistry DFT study of N ₂ O functionalization for the preparation of triazopyridine and triazoloquinoline scaffolds. Organic Chemistry Frontiers, 2022, 9, 4347-4357. | 2.3 | 7 |
| 16547 | DFT and TD-DFT Calculations of Orbital Energies and Photovoltaic Properties of Small Molecule Donor and Acceptor Materials Used in Organic Solar Cells. Journal of Renewable Materials, 2022, 10, 2553-2567. | 1.1 | 5 |
| 16548 | Non-Covalent Interactions Atlas benchmark data sets 5: London dispersion in an extended chemical space. Physical Chemistry Chemical Physics, 2022, 24, 14780-14793. | 1.3 | 26 |
| 16549 | Distortion-driven spin switching in electron-doped metal porphyrins. Journal of Materials Chemistry C, 2022, 10, 9748-9757. | 2.7 | 5 |
| 16550 | Dithienyl-naphthalenes and quaterthiophenes substituted with electron-withdrawing groups as n-type organic semiconductors for organic field-effect transistors. Journal of Materials Chemistry C, 2022, 10, 10058-10074. | 2.7 | 3 |
| 16551 | Near-surface centers of luminescence in titanium dioxide. AIP Conference Proceedings, 2022, , . | 0.3 | 1 |
| 16552 | A transferable prediction model of molecular adsorption on metals based on adsorbate and substrate properties. Physical Chemistry Chemical Physics, 2022, 24, 16545-16555. | 1.3 | 3 |
| 16553 | Nhc-Catalyzed [3+4] Annulation between 2-Dromoenal and Aryl 1,2-Diamine: Insights into Mechanisms, Chemo and Stereoselectivities. SSRN Electronic Journal, 0, , . | 0.4 | 0 |
| 16554 | A FOUR-NUCLEAR Ag(I) COMPLEX SUPPORTED BY A N,N- ϵ^2 ,N ϵ^3 ,P-LIGAND: SYNTHESIS, CRYSTAL AND ELECTRONIC STRUCTURE. Journal of Structural Chemistry, 2022, 63, 663-668. | 0.3 | 1 |
| 16555 | Cyclization Reaction of 3,5-Diacetyl-2,6-dimethylpyridine with Salicylic Aldehyde and Its Derivatives: Quantum-Chemical Study and Molecular Docking. Russian Journal of General Chemistry, 2022, 92, 914-924. | 0.3 | 2 |
| 16556 | Reconstruction of Electronic Structure of MOF-525 via Metalloporphyrin for Enhanced Photoelectro-Fenton Process. Catalysts, 2022, 12, 671. | 1.6 | 3 |
| 16557 | Noncovalent Interactions Involving Group 6 ϵ in Biological Systems: The Case of Molybdopterin and Tungstopterin Cofactors. Chemistry - A European Journal, 2022, 28, . | 1.7 | 21 |
| 16558 | Enhanced Fluorescence with Tunable Color in Doped Diphosphine-Protected Gold Nanoclusters. Journal of Physical Chemistry Letters, 2022, 13, 5873-5880. | 2.1 | 10 |
| 16559 | Gas-Phase Peroxyl Radical Recombination Reactions: A Computational Study of Formation and Decomposition of Tetroxides. Journal of Physical Chemistry A, 2022, 126, 4046-4056. | 1.1 | 9 |
| 16560 | Bistriazoles Connected Through a B \sim B Bridge, Synthesized by Highly Selective Dipolar Cycloaddition Reactions of a Diazido ϵ -diborane(4). Chemistry - A European Journal, 2022, 28, . | 1.7 | 2 |
| 16561 | pH-Responsive Gelation in Metallo-Supramolecular Polymers Based on the Protic Pyridinedicarboxamide Ligand. Chemistry of Materials, 2022, 34, 6155-6169. | 3.2 | 27 |
| 16562 | Palladium-Mediated CO ₂ Extrusion Followed by Insertion of Allenes: Translating Mechanistic Studies to Develop a One-Pot Method for the Synthesis of Alkenes. Organometallics, 0, , . | 1.1 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16563 | Binding of DEP domain to phospholipid membranes: More than just electrostatics. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2022, 1864, 183983. | 1.4 | 1 |
| 16564 | The enthralling effect of packing on the light emission of pyridazinone based luminophore: Crystallographic, electronic absorption and computational studies. <i>Journal of Molecular Structure</i> , 2022, 1267, 133513. | 1.8 | 4 |
| 16565 | Analytic Gradients for the Long-Range-Corrected XYG3 Type of Doubly Hybrid Density Functionals: Theory, Implementation, and Assessment. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3937-3946. | 1.1 | 1 |
| 16566 | Magnesium(II)â€ATP Complexes in 1â€Ethylâ€3â€Methylimidazolium Acetate Solutions Characterized by ³¹ Mg Î²â€Radiationâ€Detected NMR Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 0, , . | 7.2 | 1 |
| 16567 | Implementation and Validation of Constrained Density Functional Theory Forces in the CP2K Package. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4438-4446. | 2.3 | 5 |
| 16568 | Source of Rate Acceleration for Carbocation Cyclization in Biomimetic Supramolecular Cages. <i>Journal of the American Chemical Society</i> , 2022, 144, 11413-11424. | 6.6 | 15 |
| 16569 | Virtual Experiments on Real Asphaltenes: Predicting Properties Using Quantum Chemical Simulations of Structures from Non-contact Atomic Force Microscopy. <i>Energy & Fuels</i> , 2022, 36, 8714-8724. | 2.5 | 6 |
| 16570 | Computational protocol for predicting ¹⁹ F NMR chemical shifts for PFAS and connection to PFAS structure. <i>Journal of Computational Chemistry</i> , 2022, 43, 1355-1361. | 1.5 | 4 |
| 16571 | Onâ€Off Infrared Absorption of the Sâ€O Vibrational Probe of Dimethyl Sulfoxide. <i>Journal of Physical Chemistry B</i> , 2022, 126, 4501-4508. | 1.2 | 4 |
| 16572 | Gaining deeper insights into 2,5-disubstituted furan derivatives as potent Î±-glucosidase inhibitors and discovery of putative targets associated with diabetes diseases using an integrative computational approach. <i>Structural Chemistry</i> , 2023, 34, 519-538. | 1.0 | 4 |
| 16573 | Octanolâ€Water Partition Coefficients of Fluorinated Drug Molecules with Continuum Solvation Models. <i>Journal of Physical Chemistry A</i> , 0, , . | 1.1 | 3 |
| 16574 | A computational study for the reaction mechanism of AIBNâ€induced remote trifluoromethylâ€alkynylation of thioalkynes. <i>Journal of Physical Organic Chemistry</i> , 0, , . | 0.9 | 0 |
| 16575 | Stabilizing a 20-Electron Metallaazulyne by Aromaticity. <i>Inorganic Chemistry</i> , 2022, 61, 9073-9081. | 1.9 | 3 |
| 16576 | Green synthesis of Ag ₂ O nanoparticles using Punica granatum leaf extract for sulfamethoxazole antibiotic adsorption: characterization, experimental study, modeling, and DFT calculation. <i>Environmental Science and Pollution Research</i> , 2023, 30, 81352-81369. | 2.7 | 24 |
| 16577 | Theoretical exploration of the reactivity of cellulose models under nonâ€thermal plasma conditionsâ€mechanistic and NBO studies. <i>Journal of Computational Chemistry</i> , 2022, 43, 1334-1341. | 1.5 | 1 |
| 16578 | The mechanism of biochemical NOâ€sensing: insights from computational chemistry. <i>Chemistry - A European Journal</i> , 0, , . | 1.7 | 1 |
| 16579 | Fluorinated copper phthalocyanine as an electron transport material in perovskite solar cell. <i>International Journal of Energy Research</i> , 2022, 46, 15127-15142. | 2.2 | 15 |
| 16580 | Magnesium(II)â€ATP Complexes in 1â€Ethylâ€3â€Methylimidazolium Acetate Solutions Characterized by ³¹ Mg Î²â€Radiationâ€Detected NMR Spectroscopy. <i>Angewandte Chemie</i> , 0, , . | 1.6 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16581 | Synthesis, Characterization, DFT and Photocatalytic Studies of a New Pyrazine Cadmium(II) Tetrakis(4-methoxy-phenyl)-porphyrin Compound. <i>Molecules</i> , 2022, 27, 3833. | 1.7 | 4 |
| 16582 | Comprehensive Quantum Chemical Characterization of the Astrochemically Relevant HC _n Chain Family: An Attempt to Aid Astronomical Observations. <i>Advanced Theory and Simulations</i> , 2022, 5, . | 1.3 | 8 |
| 16583 | Importance of an Axial Ln ^{III} –F Bond across the Lanthanide Series and Single-Molecule Magnet Behavior in the Ce and Nd Analogues. <i>Inorganic Chemistry</i> , 2022, 61, 9906-9917. | 1.9 | 6 |
| 16584 | Reaction of Ta ₃ ⁺ Clusters with Molecular Nitrogen: A Mechanism Investigation. <i>ACS Omega</i> , 2022, 7, 22682-22688. | 1.6 | 3 |
| 16585 | Compression Produces a Square-Planar Iron Tetracarbonyl. <i>Inorganic Chemistry</i> , 2022, 61, 9055-9062. | 1.9 | 1 |
| 16586 | Photochemical Deracemization of Chiral Alkenes via Triplet Energy Transfer. <i>Journal of the American Chemical Society</i> , 2022, 144, 10133-10138. | 6.6 | 34 |
| 16587 | Electrochemical Study of Vicinal Dibromide Dehalogenation Catalyzed by Cobaloximes. <i>Journal of the Electrochemical Society</i> , 2022, 169, 063518. | 1.3 | 1 |
| 16588 | Revealing the regioselective N-acylation of 5-bromo-2-aminobenzimidazole using experiment and theoretical calculation. <i>Tetrahedron</i> , 2022, , 132905. | 1.0 | 1 |
| 16589 | C–H and Si–H Activation Reactions at Ru/Ga Complexes: A Combined Experimental and Theoretical Case Study on the Ru–Ga Bond. <i>Chemistry - A European Journal</i> , 2022, 28, . | 1.7 | 6 |
| 16590 | Describing Chemical Reactivity with Frontier Molecular Orbitals. <i>Jacs Au</i> , 2022, 2, 1383-1394. | 3.6 | 32 |
| 16591 | Machine Learning Models Predict Calculation Outcomes with the Transferability Necessary for Computational Catalysis. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4282-4292. | 2.3 | 9 |
| 16592 | Highly Efficient Blue Thermally Activated Delayed Fluorescence Emitters Based on Multi-Donor Modified Oxygen-Bridged Boron Acceptor. <i>Molecules</i> , 2022, 27, 4048. | 1.7 | 3 |
| 16593 | A step-by-step investigation of sodium chloride clusters: accurate references, assessment of low-cost methods, and convergence from molecule to salt. <i>Molecular Physics</i> , 2023, 121, . | 0.8 | 4 |
| 16594 | Study the application of new type green corrosion inhibitors for iron metal. <i>Inorganic Chemistry Communication</i> , 2022, 142, 109650. | 1.8 | 6 |
| 16595 | Theoretical Study of Mechanism and Product Selectivity of Metal-Catalyzed Reactions of Alkynyl Thioethers with Isoxazoles/Anthranils. <i>Molecular Catalysis</i> , 2022, 528, 112432. | 1.0 | 0 |
| 16596 | Weak antiferromagnetic interaction in Cu(II) complex with semi-coordination exchange pathway. <i>Polyhedron</i> , 2022, 223, 115962. | 1.0 | 6 |
| 16597 | Enol or keto? Interplay between solvents and substituents as a factor controlling ESPT. <i>Journal of Molecular Liquids</i> , 2022, 361, 119611. | 2.3 | 9 |
| 16598 | Photophysical, catalytic, and theoretical investigations of kinetically stable [Cu(2,2'-biquinoline)(PR ₃) ₂] ⁺ and [Cu(neocuproine)(PR ₃) ₂] ⁺ complexes. <i>Polyhedron</i> , 2022, 224, 115975. | 1.0 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16599 | Flexible and free-standing bacterial cellulose derived cathode host and separator for lithium-sulfur batteries. <i>Carbohydrate Polymers</i> , 2022, 293, 119731. | 5.1 | 22 |
| 16600 | Synthesis and characterization of a series of cobalt complexes: Investigation of their efficacy as sensitizers in dye-sensitized solar cell applications. <i>Journal of Molecular Structure</i> , 2022, 1266, 133512. | 1.8 | 4 |
| 16601 | Exploring competitive inhibition of a family 10 xylanase derived from Hu sheep rumen microbiota by <i>Oryza sativa</i> xylanase inhibitor protein: In vitro and in silico perspectives. <i>Enzyme and Microbial Technology</i> , 2022, 160, 110082. | 1.6 | 5 |
| 16602 | Characteristics of graphite oxide membranes with different thickness by low temperature thermal reduction for aqueous EDLC electrodes and hot activation phenomenon. <i>Materials Research Bulletin</i> , 2022, 154, 111927. | 2.7 | 2 |
| 16603 | Ultrafast FÅrster resonance energy transfer between tyrosine and tryptophan: potential contributions to proteinâ€“water dynamics measurements. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18055-18066. | 1.3 | 4 |
| 16604 | A Structure and Electronics Study into Ferrocene Alkene Compounds Produced from Organic Acids. <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 0 |
| 16605 | An induced-fit model for asymmetric organocatalytic reactions: a case study of the activation of olefins <i>via</i> chiral BrÅnsted acid catalysts. <i>Chemical Science</i> , 2022, 13, 8848-8859. | 3.7 | 8 |
| 16606 | An organic transistor for the selective detection of tropane alkaloids utilizing a molecularly imprinted polymer. <i>Journal of Materials Chemistry B</i> , 2022, 10, 6808-6815. | 2.9 | 9 |
| 16607 | Voltage Prediction of Vanadium Redox Flow Batteries from First Principles. <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 0 |
| 16608 | Understanding the effect of the exchange-correlation functionals on methane and ethane formation over ruthenium catalysts. <i>Chinese Journal of Chemical Physics</i> , 0, , . | 0.6 | 1 |
| 16609 | Towards a relationship between photoluminescence emissions and photocatalytic activity of Ag₂SeO₄: combining experimental data and theoretical insights. <i>Dalton Transactions</i> , 2022, 51, 11346-11362. | 1.6 | 5 |
| 16610 | Exploration of the photocatalytic cycle for sacrificial hydrogen evolution by conjugated polymers containing heteroatoms. <i>Sustainable Energy and Fuels</i> , 2022, 6, 3756-3767. | 2.5 | 2 |
| 16611 | The nature of metalâ€“metal bonding in Re-, Ru- and Os-corrole dimers. <i>RSC Advances</i> , 2022, 12, 18728-18735. | 1.7 | 1 |
| 16612 | One-Electron Transfer during Dimerization of Phenoxy Radicals. <i>Russian Journal of Organic Chemistry</i> , 2022, 58, 637-647. | 0.3 | 0 |
| 16613 | New insights into the deterioration of TiO2 based oil paints: the effects of illumination conditions and surface interactions. <i>Heritage Science</i> , 2022, 10, . | 1.0 | 5 |
| 16614 | Following the density evolution using real time density functional theory and density based indexes: Application to model pushâ€“pull molecules. <i>Journal of Computational Chemistry</i> , 2022, 43, 1464-1473. | 1.5 | 3 |
| 16615 | A local hybrid exchange functional approximation from first principles. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 18 |
| 16616 | Computation of Oxidation Potentials of Solvated Nucleobases by Static and Dynamic Multilayer Approaches. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3365-3380. | 2.5 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 16617 | Wide Nematogenic Azomethine/Ester Liquid Crystals Based on New Biphenyl Derivatives: Mesomorphic and Computational Studies. <i>Molecules</i> , 2022, 27, 4150. | 1.7 | 18 |
| 16618 | Delayed Fluorescence by Triplet-Triplet Annihilation from Columnar Liquid Crystal Films. <i>ACS Applied Electronic Materials</i> , 2022, 4, 3486-3494. | 2.0 | 2 |
| 16619 | Decorated Decoration of a Tetraazaperylene with Urea Units: Chiral Octaazaperopyrenedioxides (OAPPDOs) and Their Optical and Chiroptical Properties. <i>Chemistry - A European Journal</i> , 2022, 28, . | 1.7 | 9 |
| 16620 | A Computational Study on Phenylboronic Acid-Pillared Graphene Oxide Frameworks for Gas Storage and Separation. <i>ACS Applied Nano Materials</i> , 2022, 5, 9286-9297. | 2.4 | 2 |
| 16621 | Supramolecular cis-Bis(Chelation) of $[M(CN)_6]^{3-}$ (M = CrIII, FeIII, CoIII) by Phloroglucinol (H3PG). <i>Molecules</i> , 2022, 27, 4111. | 1.7 | 1 |
| 16622 | Modeling Heme Peroxidase: Heme Saddling Facilitates Reactions with Hyperperoxides to Form High-Valent Fe(IV)-Oxo Species. <i>Chemistry - A European Journal</i> , 0, , . | 1.7 | 1 |
| 16623 | Oriented External Electric Fields Regulating the Reaction Mechanism of CH ₄ Oxidation Catalyzed by Fe(IV)-Oxo-Corrolazine: Insight from Density Functional Calculations. <i>Frontiers in Chemistry</i> , 0, 10, . | 1.8 | 3 |
| 16624 | Mechanistic Insight into the Ni-Catalyzed Kumada Cross-Coupling: Alkylmagnesium Halide Promotes C-F Bond Activation and Electron-Deficient Metal Center Slows Down β -H Elimination. <i>Journal of Organic Chemistry</i> , 2022, 87, 8902-8909. | 1.7 | 7 |
| 16625 | Benchmarking time-dependent density functional theory predictions of emission spectra and color: A rainbow of error. <i>International Journal of Quantum Chemistry</i> , 0, , . | 1.0 | 1 |
| 16626 | Coupled Cluster Benchmarking of Large Noncovalent Complexes in L7 and S12L as Well as the C ₆₀ Dimer, DNA-Ellipticine, and HIV-Indinavir. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4326-4341. | 1.1 | 11 |
| 16627 | Spatial and Temporal Resolution of the Oxygen-Independent Photoinduced DNA Interstrand Cross-Linking by a Nitroimidazole Derivative. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3239-3252. | 2.5 | 6 |
| 16628 | Rotational Spectroscopy of the 2,2,3,3-Pentafluoropropanol...Water Complex: Conformations and Large Amplitude Motions. <i>ChemPhysChem</i> , 2022, 23, . | 1.0 | 3 |
| 16629 | H ₂ O-Boosted Mg ²⁺ /Proton Collaborated Energy Storage for Rechargeable Mg-Metal Batteries. <i>Advanced Energy Materials</i> , 2022, 12, . | 10.2 | 6 |
| 16630 | Preparation of photonic molecular trains via soft-crystal polymerization of lanthanide complexes. <i>Nature Communications</i> , 2022, 13, . | 5.8 | 7 |
| 16631 | Insight into the Crystal Structures and Potential of Two Newly Synthesized Naproxen-Based Hydrazide Derivatives as Potent COX-2 Inhibitors. <i>Applied Biochemistry and Biotechnology</i> , 0, , . | 1.4 | 1 |
| 16632 | Parallelized Raman Difference Spectroscopy for the Investigation of Chemical Interactions. <i>Analytical Chemistry</i> , 2022, 94, 10346-10354. | 3.2 | 8 |
| 16633 | Spin-active defects in hexagonal boron nitride. <i>Materials for Quantum Technology</i> , 2022, 2, 032002. | 1.2 | 18 |
| 16634 | Quantum computing in pharma: A multilayer embedding approach for near future applications. <i>Journal of Computational Chemistry</i> , 2023, 44, 406-421. | 1.5 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16635 | Nickel-Catalyzed Enantioselective Reductive Alkyl-Carbamoylation of Internal Alkenes. <i>Angewandte Chemie</i> , 0, . | 1.6 | 0 |
| 16636 | Nickel-Catalyzed Enantioselective Reductive Alkyl-Carbamoylation of Internal Alkenes. <i>Angewandte Chemie - International Edition</i> , 2022, 61, . | 7.2 | 17 |
| 16637 | 3D and 2D aromatic units behave like oil and water in the case of benzocarborane derivatives. <i>Nature Communications</i> , 2022, 13, . | 5.8 | 23 |
| 16638 | Exploiting Ligand Additivity for Transferable Machine Learning of Multireference Character across Known Transition Metal Complex Ligands. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4836-4845. | 2.3 | 4 |
| 16639 | New Carbamates and Ureas: Comparative Ability to Gel Organic Solvents. <i>Gels</i> , 2022, 8, 440. | 2.1 | 1 |
| 16640 | Energetic triazinium salts from N-amination of 3,5-diamino-6-nitro-1,2,4-triazine. <i>Energetic Materials Frontiers</i> , 2022, 3, 128-136. | 1.3 | 3 |
| 16641 | Delocalization error: The greatest outstanding challenge in density-functional theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2023, 13, . | 6.2 | 43 |
| 16642 | Hypervalent Chalcogenonium-Coordination Bonding Catalysis. <i>Angewandte Chemie</i> , 0, . | 1.6 | 0 |
| 16643 | Three-Dimensional Quantitative Structure and Activity Relationship of Flavones on Their Hypochlorite Scavenging Capacity. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 8799-8807. | 2.4 | 3 |
| 16644 | Density functional theory calculations of ^{13}C and ^1H chemical shifts and $^3\text{J}(\text{C}^{13}-\text{O}^1-\text{O}^1-\text{C}^1)$ coupling constants as structural and analytical tools in hydroperoxides: Prospects and limitations of $^1\text{H}-^{13}\text{C}$ heteronuclear multiple bond correlation experiments. <i>Magnetic Resonance in Chemistry</i> , 2022, 60, 870-884. | 1.1 | 4 |
| 16645 | Synthesis, quantum mechanical calculations, molecular docking, Hirshfeld surface analysis and ADMET estimation studies of (E)-3-(anthracene-10-yl)-1-(naphthalen-1-yl)prop-2-en-1-one. <i>Journal of Molecular Structure</i> , 2022, , 133748. | 1.8 | 0 |
| 16646 | Molecular properties and tautomeric equilibria of isolated flavins. <i>Journal of Computational Chemistry</i> , 0, . | 1.5 | 1 |
| 16647 | A Look at Real-World Transition-Metal Thermochemistry and Kinetics with Local Hybrid Functionals. <i>Israel Journal of Chemistry</i> , 2023, 63, . | 1.0 | 8 |
| 16649 | Solvent promoted tautomerism in thione-containing tetraazatricyclics: evidence from ^1H NMR spectroscopy and transition state studies. <i>Journal of Molecular Modeling</i> , 2022, 28, . | 0.8 | 1 |
| 16650 | From Mosaic-Type to Heterojunction-Type SEI Films on the Li Anode: Decoupling Chemical and Electrochemical Degradation of the Electrolyte. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 9232-9241. | 3.2 | 4 |
| 16651 | Density functional theory studies of polypyrrole and polypyrrole derivatives; substituent effect on the optical and electronic properties. <i>Polymer</i> , 2022, 255, 125127. | 1.8 | 9 |
| 16652 | Adsorption of CO_2 , H_2O , H_2S , NH_3 and NO_2 on germanane nanosheet-A density functional study. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113799. | 1.1 | 5 |
| 16653 | Green fruit organic primary battery: Positive citric acid, negative sodium tert-pentoxide. <i>Journal of Electroanalytical Chemistry</i> , 2022, 920, 116582. | 1.9 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 16654 | Synergetic electron donation and back-donation interactions in (Au ⁺ CO ₂) ⁻ complex: A joint anionic photoelectron velocity-map imaging spectroscopy and theoretical investigation. <i>Chemical Physics Letters</i> , 2022, 803, 139845. | 1.2 | 0 |
| 16655 | Enhanced photovoltaic performance of D-π-A organic sensitizers by simple fluorination of acceptor unit. <i>Organic Electronics</i> , 2022, 108, 106606. | 1.4 | 0 |
| 16656 | Synthesis, structure and reactivity of a boron-containing spirocycle carbanion. <i>Inorganic Chemistry Communication</i> , 2022, 143, 109728. | 1.8 | 0 |
| 16657 | Strain-Induced asymmetry and on-site dynamics of silicon defects in graphene. <i>Carbon Trends</i> , 2022, 9, 100189. | 1.4 | 0 |
| 16658 | Deep removal of chlorobenzene based volatile organic compounds from exhaust gas with ionic liquids. <i>Separation and Purification Technology</i> , 2022, 298, 121610. | 3.9 | 17 |
| 16659 | Bicyclic thiaspiro[4.n]alkanones: Investigating their total stereochemistry achieved by the catalyst-free sulfa-Michael reaction. <i>Journal of Molecular Structure</i> , 2022, 1267, 133617. | 1.8 | 0 |
| 16660 | Calculation of Gas-phase Standard Formation Enthalpy via Ring-Preserved Connectivity-Based Hierarchy and Automatic Bond Separation Reaction Platform. <i>Fuel</i> , 2022, 327, 125203. | 3.4 | 7 |
| 16661 | Optofluidic analysis of monolayers with infrared microscopy. , 2023, , . | | 0 |
| 16662 | Investigation Study of Molecular Modeling for New Pt(IV) Complex Using Density Functional Theory. <i>Arab Gulf Journal of Scientific Research</i> , 2016, , 69-78. | 0.3 | 0 |
| 16663 | Singlet-triplet energy gap of multiresonant molecular systems: A double hybrid time-dependent density functional theory study. <i>Chemical Physics Letters</i> , 2022, 804, 139895. | 1.2 | 3 |
| 16664 | Mechanistic Details of the Sharpless Epoxidation of Allylic Alcohols—A Combined URVA and Local Mode Study. <i>Catalysts</i> , 2022, 12, 789. | 1.6 | 4 |
| 16665 | A unique colorimetric and ratiometric reversible fluorescent probe for HSO ₃ ⁻ /H ₂ O ₂ detection and imaging in real water samples, rice leaves and roots. <i>Dyes and Pigments</i> , 2022, 205, 110591. | 2.0 | 7 |
| 16666 | Fullerenes Pose a Strain on Hybrid Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4709-4720. | 1.1 | 5 |
| 16667 | Electronic Structure of Molecular Cobalt Catalysts for H ₂ Production Revealed by Multifrequency EPR. <i>Journal of Physical Chemistry C</i> , 2022, 126, 11889-11899. | 1.5 | 0 |
| 16668 | Superionic Bifunctional Polymer Electrolytes for Solid-State Energy Storage and Conversion. <i>Advanced Materials</i> , 2023, 35, . | 11.1 | 13 |
| 16669 | Bucket Effect to Improve ^{Third-Order} Nonlinear Optical Response on ^{Metal-Heteroaromatic} Compounds. <i>Chinese Journal of Chemistry</i> , 2022, 40, 2611-2617. | 2.6 | 6 |
| 16670 | Unveiling the sensing mechanism and luminescence property of a new ESIPT-based fluorescent sensor for detecting Zn ²⁺ . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 282, 121650. | 2.0 | 16 |
| 16671 | Hypervalent Chalcogenoniumâ€¦â€¦â€¦ Bonding Catalysis. <i>Angewandte Chemie - International Edition</i> , 2022, 61, 7:2 | | 12 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16672 | Conformational distributions of helical perfluoroalkyl substances and impacts on stability. Journal of Computational Chemistry, 2022, 43, 1656-1661. | 1.5 | 8 |
| 16673 | Radial Kohn-Sham problem via integral-equation approach. Journal of Physics Communications, 2022, 6, 085002. | 0.5 | 1 |
| 16674 | Spectroscopic investigation and density functional theory prediction of first and second order hyperpolarizabilities of 1-(4-bromophenyl)-3-(2,4-dichlorophenyl)prop-2-en-1-one. Journal of Molecular Structure, 2022, 1269, 133807. | 1.8 | 4 |
| 16675 | NMR and computational studies of ammonium ion binding to dibenzo-18-crown-6. Structural Chemistry, 0, , . | 1.0 | 0 |
| 16676 | DFT Investigation of Polyethylene-co-vinyl Acetate: Kinetics of Initiation and Propagation, Copolymer Composition, and Unit Sequence Distribution. Industrial & Engineering Chemistry Research, 2022, 61, 10775-10789. | 1.8 | 2 |
| 16677 | Novel Zinc(II) and Copper(II) Complexes of 2-((2-Hydroxyethyl)amino)quinoline-3-carbaldehyde for Antibacterial and Antioxidant Activities: A Combined Experimental, DFT, and Docking Studies. ACS Omega, 2022, 7, 26336-26352. | 1.6 | 22 |
| 16678 | Tuning of Thermometric Performances of Mixed Eu-Tb Metal-Organic Frameworks through Single-Crystal Coordinating Solvent Exchange Reactions. Advanced Optical Materials, 2022, 10, . | 3.6 | 6 |
| 16679 | Structural and magnetic characterization of mixed-valence vanadium (IV/V) complex with $\{(VO)_2(\mu^2-O)\}_3^+$ core: Theoretical and experimental insights. Journal of Molecular Structure, 2022, 1269, 133805. | 1.8 | 8 |
| 16680 | Sequential and concerted C-C and C-O bond dissociation in the Coulomb explosion of 2-propanol. Journal of Chemical Physics, 2022, 157, . | 1.2 | 4 |
| 16681 | Molecular Electrides: An In Silico Perspective. ChemPhysChem, 2022, 23, . | 1.0 | 4 |
| 16682 | Effective absorption of dichloromethane using deep eutectic solvents. Journal of Hazardous Materials, 2022, 439, 129666. | 6.5 | 19 |
| 16683 | Design and synthesis of novel heterocyclic pivalamide ligands and their copper(II) complexes: Structure, BSA/DNA interactions and SOD synzyme activity. Polyhedron, 2022, 225, 116054. | 1.0 | 4 |
| 16684 | Copper complexes of strongly electron rich and deficient salen ligands. Inorganica Chimica Acta, 2022, 542, 121106. | 1.2 | 4 |
| 16685 | A niobium pentafulvene ethylene complex: synthesis, properties and reaction pathways. Dalton Transactions, 2022, 51, 12502-12511. | 1.6 | 3 |
| 16686 | Investigation on Molecular Dynamics Simulation for Predicting Kinematic Viscosity of Natural Ester Insulating Oil. IEEE Transactions on Dielectrics and Electrical Insulation, 2022, 29, 1882-1888. | 1.8 | 7 |
| 16687 | A graph representation of molecular ensembles for polymer property prediction. Chemical Science, 2022, 13, 10486-10498. | 3.7 | 41 |
| 16688 | Understanding ion diffusion in anion exchange membranes; effects of morphology and mobility of pendant cationic groups. Journal of Materials Chemistry A, 2022, 10, 18295-18307. | 5.2 | 13 |
| 16689 | Stable, Bright, and Long-Fluorescence-Lifetime Dyes for Deep-Near-Infrared Bioimaging. Journal of the American Chemical Society, 2022, 144, 14351-14362. | 6.6 | 65 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16690 | Photochemical and thermochemical pathways to S ₂ and polysulfur formation in the atmosphere of Venus. <i>Nature Communications</i> , 2022, 13, . | 5.8 | 4 |
| 16691 | STRUCTURE - THERMAL PROPERTIES RELATIONSHIP IN VOLATILE HETEROMETALLIC COMPLEXES USED IN CVD OF Cu-Pt AND Cu-Pd FILMS. <i>Journal of Structural Chemistry</i> , 2022, 63, 1070-1078. | 0.3 | 0 |
| 16692 | Novel Prediction Model of Band Gap in Organic-Inorganic Hybrid Perovskites Based on a Simple Cluster Model Database. <i>Journal of Physical Chemistry C</i> , 2022, 126, 13409-13415. | 1.5 | 6 |
| 16693 | Nucleotide Recognition by a Guanidinocalixarene Receptor in Aqueous Solution. <i>Chemical Research in Chinese Universities</i> , 2023, 39, 144-150. | 1.3 | 4 |
| 16694 | Nanocluster of Aluminum Lattice via Organic Inhibitors Coating: A Study of Freundlich Adsorption. <i>Journal of Cluster Science</i> , 2023, 34, 1547-1562. | 1.7 | 16 |
| 16695 | Anomalous Infrared Absorbance of S ₂ O: A Perturbation Study of \hat{I}_{\pm} -C ⁺ H/D. <i>Journal of Physical Chemistry B</i> , 2022, 126, 5490-5496. | 1.2 | 2 |
| 16696 | Recent Advances in Cartesian-Grid DFT in Atoms and Molecules. <i>Frontiers in Chemistry</i> , 0, 10, . | 1.8 | 0 |
| 16697 | High-Level Quantum Chemistry Reference Heats of Formation for a Large Set of C, H, N, and O Species in the NIST Chemistry Webbook and the Identification and Validation of Reliable Protocols for Their Rapid Computation. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4981-4990. | 1.1 | 13 |
| 16698 | Advancing the Am Extractant Design through the Interplay among Planarity, Preorganization, and Substitution Effects. <i>Inorganic Chemistry</i> , 2022, 61, 11556-11570. | 1.9 | 11 |
| 16699 | Electron Attachment to 5-Fluorouracil: The Role of Hydrogen Fluoride in Dissociation Chemistry. <i>International Journal of Molecular Sciences</i> , 2022, 23, 8325. | 1.8 | 7 |
| 16700 | Insights into the Capture of CO ₂ by Nickel Hydride Complexes. <i>Catalysts</i> , 2022, 12, 790. | 1.6 | 3 |
| 16701 | Proton Relay Effects on Oxygen Reduction Reaction Catalyzed by Dinuclear Cobalt Polypyridyl Complexes with OH Groups on Bipyridine Ligands. <i>Bulletin of the Chemical Society of Japan</i> , 2022, 95, 1100-1110. | 2.0 | 1 |
| 16702 | Complexation of Astatine(III) with Ketones: Roles of NO ₃ ⁻ Counterion and Exploration of Possible Binding Modes. <i>Inorganic Chemistry</i> , 2022, 61, 12087-12096. | 1.9 | 8 |
| 16703 | Insertion of Carbon Monoxide into the Terminal Co-O Bond in a Methoxocobalt(III) Complex via a Tuneable Mechanism. <i>Organometallics</i> , 2022, 41, 2220-2226. | 1.1 | 2 |
| 16704 | Solvent Organization and Electrostatics Tuned by Solute Electronic Structure: Amide versus Non-Amide Carbonyls. <i>Journal of Physical Chemistry B</i> , 2022, 126, 5876-5886. | 1.2 | 3 |
| 16705 | Lubricant hydrogenation over a functionalized clay-based Pd catalyst: A combined computational and experimental study. <i>Applied Organometallic Chemistry</i> , 2022, 36, . | 1.7 | 7 |
| 16706 | Theoretical Study of the Electrochemical Properties for Solid Electrolytes Containing Ethoxy and Carbonate Groups. <i>Journal of the Electrochemical Society</i> , 2022, 169, 080519. | 1.3 | 1 |
| 16707 | Substituent Control of Near-Infrared Absorption of Triphenylamine Radical Cation. <i>Colorants</i> , 2022, 1, 354-362. | 0.9 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 16708 | Design and Development of Benzothiazole-Based Fluorescent Probes for Selective Detection of A β 2 Aggregates in Alzheimer's Disease. ACS Chemical Neuroscience, 2022, 13, 2503-2516. | 1.7 | 14 |
| 16709 | Trigonal Planar Au@Ag ₃ Clusters Showing Exceptionally Fast and Efficient Phosphorescence in Violet to Deep-Blue Region. Chemistry - A European Journal, 2022, 28, . | 1.7 | 4 |
| 16710 | High performance computing for first-principles Kohn-Sham density functional theory towards exascale supercomputers. CCF Transactions on High Performance Computing, 2023, 5, 26-42. | 1.1 | 1 |
| 16711 | Adsorption and Activation of O ₂ on Small Gold Oxide Clusters: the Reactivity Dominated by Site-Specific Factors. Journal of Physical Chemistry A, 2022, 126, 5594-5603. | 1.1 | 2 |
| 16712 | Applications of a perturbation-aware local correlation method to coupled cluster linear response properties. Molecular Physics, 0, , . | 0.8 | 1 |
| 16713 | Intramolecular force field for carboxylate Pt(II)-complexes. Theoretical Chemistry Accounts, 2022, 141, . | 0.5 | 1 |
| 16714 | Experimental and Theoretical Analysis of Synthesized Poly(Pthalazinone Ether Sulfone Ketone) Copolymer-Modified Separators for Li-S Batteries. ChemElectroChem, 2022, 9, . | 1.7 | 1 |
| 16715 | Electroinduced crosslinking of triphenylamine-based polybenzoxazines. Microchemical Journal, 2022, 182, 107878. | 2.3 | 4 |
| 16716 | Computational Prediction of Tc-99 NMR Chemical Shifts in Technetium Complexes with Radiopharmaceutical Applications. Journal of Physical Chemistry A, 2022, 126, 5434-5448. | 1.1 | 3 |
| 16717 | Discovery of Ircinianin Lactones B and C—Two New Cyclic Sesterterpenes from the Marine Sponge Ircinia wistarii. Marine Drugs, 2022, 20, 532. | 2.2 | 4 |
| 16718 | Structural and bonding properties of gas-phase M ₄ C ₆ (M = Cu, Ag, and Au) clusters and their anions. Molecular Physics, 0, , . | 0.8 | 0 |
| 16719 | An assessment of orbital energy corrections for the direct random phase approximation and explicit <i>i</i> -functionals. Molecular Physics, 0, , . | 0.8 | 5 |
| 16720 | Computational Biomaterials: Computational Simulations for Biomedicine. Advanced Materials, 2023, 35, . | 11.1 | 10 |
| 16721 | Benchmarking time-dependent density functional theory for singlet excited states of thermally activated delayed fluorescence chromophores. Physical Review Research, 2022, 4, . | 1.3 | 10 |
| 16722 | Disentangling the electronic structure of an adsorbed graphene nanoring by scanning tunneling microscopy. Communications Materials, 2022, 3, . | 2.9 | 2 |
| 16724 | QM/MM Well-Tempered Metadynamics Study of the Mechanism of XBP1 mRNA Cleavage by Inositol Requiring Enzyme 1 \pm RNase. Journal of Chemical Information and Modeling, 2022, 62, 4247-4260. | 2.5 | 3 |
| 16725 | Molecular dynamics insight into phase separation and transport in anion-exchange membranes: Effect of hydrophobicity of backbones. Journal of Membrane Science, 2022, 661, 120922. | 4.1 | 28 |
| 16726 | Spectrochemistry of Firefly Bioluminescence. Chemical Reviews, 2022, 122, 13207-13234. | 23.0 | 24 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16728 | The Speciation of Americium Cations in Neat Water Implicated from DFT Studies. <i>Inorganic Chemistry</i> , 2022, 61, 13858-13867. | 1.9 | 1 |
| 16729 | Dual-Level Training of Gaussian Processes with Physically Inspired Priors for Geometry Optimizations. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 5739-5754. | 2.3 | 5 |
| 16730 | Pyrolysis of mass-selected (V ₂ O ₅) _n O ⁺ (<i>n</i> = 1–6) clusters in a high-temperature linear ion trap reactor. <i>Journal of Chemical Physics</i> , 2022, 157, 114301. | 1.2 | 5 |
| 16731 | Vat Orange 7 as an organic electrode with ultrafast hydronium-ion storage and super-long life for rechargeable aqueous zinc batteries. <i>Chemical Engineering Journal</i> , 2023, 451, 138776. | 6.6 | 10 |
| 16732 | Generalized oscillator strength of the core-excited states of molecular nitrogen studied by nonresonant inelastic x-ray scattering. <i>Physical Review A</i> , 2022, 106, . | 1.0 | 0 |
| 16733 | Effect of bridging units on the photophysical properties of ⁴Eu ²⁺ appended salen [−] indium complexes. <i>Bulletin of the Korean Chemical Society</i> , 2022, 43, 1177-1183. | 1.0 | 2 |
| 16734 | Benefits of Range-Separated Hybrid and Double-Hybrid Functionals for a Large and Diverse Data Set of Reaction Energies and Barrier Heights. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5492-5505. | 1.1 | 11 |
| 16735 | One-Step Catalytic Activation Promoting Pore Development of Zhundong Coal-Based Activated Coke: A Compared Study with Conventional Carbonization–Activation Combined Process. <i>Energy & Fuels</i> , 2022, 36, 9171-9181. | 2.5 | 6 |
| 16736 | DFT-1/2 and shell DFT-1/2 methods: electronic structure calculation for semiconductors at LDA complexity. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 403001. | 0.7 | 17 |
| 16737 | Fiber swelling to improve cycle performance of paper-based separator for lithium-ion batteries application. <i>Journal of Energy Chemistry</i> , 2023, 79, 92-100. | 7.1 | 11 |
| 16738 | Molecularly Imprinted Nanoparticles towards MMP9 for Controlling Cardiac ECM after Myocardial Infarction: A Predictive Experimental-Computational Chemistry Investigation. <i>Biomedicines</i> , 2022, 10, 2070. | 1.4 | 3 |
| 16739 | Choice of computational protocol for carbon–lithium spin–spin coupling constants ¹J_{CLi}. <i>Magnetic Resonance in Chemistry</i> , 2022, 60, 985-995. | 1.1 | 3 |
| 16740 | Machine-learning assisted design principle search for singlet fission: an example study of cibalackrot. <i>Npj Computational Materials</i> , 2022, 8, . | 3.5 | 7 |
| 16741 | Computational Studies of the Photodegradation Mechanism of the Highly Phototoxic Agent Benoxaprofen. <i>ACS Omega</i> , 2022, 7, 29475-29482. | 1.6 | 1 |
| 16742 | Protonated Î±-N-Acetyl Galactose Glycopeptide Dissociation Chemistry. <i>Journal of the American Society for Mass Spectrometry</i> , 0, , . | 1.2 | 1 |
| 16743 | Accurate theoretical evaluation of strain energy of all-carboatomic ring (cyclo[2n]carbon), boron nitride ring, and cyclic polyacetylene. <i>Chinese Physics B</i> , 2022, 31, 126101. | 0.7 | 9 |
| 16744 | Revealing dissolution behavior and thermodynamic properties of tinidazole in 12 mono-solvents based on experiments and molecular simulation. <i>Journal of Molecular Liquids</i> , 2022, 366, 120081. | 2.3 | 4 |
| 16745 | Efficient Implementation of Block-Correlated Coupled Cluster Theory Based on the Generalized Valence Bond Reference for Strongly Correlated Systems. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 5276-5285. | 2.3 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 16746 | Unusual Enantiodivergence in Chiral Brønsted Acid-Catalyzed Asymmetric Allylation with α -Alkenyl Allylic Boronates. <i>Angewandte Chemie</i> , 0, , . | 1.6 | 0 |
| 16747 | Spectroscopic analysis (FT-IR/FT-Raman), electronic (UV-vis), NMR and docking on 4-methoxyphenylboronic acid (4MPBA) by DFT calculation. <i>Molecular Crystals and Liquid Crystals</i> , 2023, 755, 23-40. | 0.4 | 2 |
| 16748 | Why Ortho- and Para-Hydroxy Metabolites Can Scavenge Free Radicals That the Parent Atorvastatin Cannot? Important Pharmacologic Insight from Quantum Chemistry. <i>Molecules</i> , 2022, 27, 5036. | 1.7 | 4 |
| 16749 | Formation of phosphorus monoxide through the $\text{P}(\text{S})_4 + \text{O} \rightarrow \text{P}(\text{O})_3 + \text{PO}$ reaction. <i>Journal of Molecular Modeling</i> , 2022, 28, . | 0.8 | 2 |
| 16750 | A Computational Protocol for Vibrational Circular Dichroism Spectra of Cyclic Oligopeptides. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5458-5471. | 1.1 | 11 |
| 16751 | Magical Molecules and a New Look at Chemical Diversity of Hydrocarbons. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 7600-7606. | 2.1 | 5 |
| 16752 | Luminescent Iridium Complexes with a Sulfurated Bipyridine Ligand: PCET Thermochemistry of the Disulfide Unit and Photophysical Properties. <i>Inorganic Chemistry</i> , 0, , . | 1.9 | 2 |
| 16753 | Carbon Nanodots from an In Silico Perspective. <i>Chemical Reviews</i> , 2022, 122, 13709-13799. | 23.0 | 45 |
| 16754 | Manipulating the rotation modes by electricity and light based on the second-generation molecular motor. <i>Applied Physics A: Materials Science and Processing</i> , 2022, 128, . | 1.1 | 0 |
| 16755 | Construction of 3,12-Diazatetracyclododecane-dienes through Unexpected Visible-Light-Induced Radical Cascade Cyclization. <i>Journal of Organic Chemistry</i> , 2022, 87, 10937-10946. | 1.7 | 2 |
| 16756 | An optimally tuned range-separated hybrid starting point for <i>ab initio</i> GW plus Bethe-Salpeter equation calculations of molecules. <i>Journal of Chemical Physics</i> , 2022, 157, 074103. | 1.2 | 14 |
| 16757 | Hardness of molecules and bandgap of solids from a generalized gradient approximation exchange energy functional. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 0 |
| 16758 | On the Reactivity of N-Substituted Imidates Towards 1,4-Bisnucleophiles: An Experimental and Theoretical Study. <i>Chemistry Africa</i> , 0, , . | 1.2 | 0 |
| 16759 | Temperature, pressure, and adsorption-dependent redox potentials: I. Processes of CO_2 reduction to value-added compounds. <i>Energy Science and Engineering</i> , 2022, 10, 4520-4543. | 1.9 | 3 |
| 16760 | Mechanistic aspects of the $\text{Pd}(\text{OAc})_2$ catalyzed ethylene acetoxylation: A density functional theory study. <i>Applied Organometallic Chemistry</i> , 2022, 36, . | 1.7 | 1 |
| 16761 | Advances and Challenges in DFT-based Energy Materials Design. <i>Chinese Physics B</i> , 0, , . | 0.7 | 8 |
| 16762 | Molecular Structure and Spectroscopic Exploration of Antiviral Drug Docosanol: a Combined Experimental and DFT Study. <i>Brazilian Journal of Physics</i> , 2022, 52, . | 0.7 | 1 |
| 16763 | Self-adaptive real-time time-dependent density functional theory for x-ray absorptions. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 16764 | Accurate Non-Adiabatic Couplings from Optimally-Tuned Range-Separated Hybrid Functionals. <i>Journal of Chemical Physics</i> , 0, , . | 1.2 | 3 |
| 16766 | Analysis of the relative stability of trigonal and tetrahedral boronate cyclic esters in terms of boronic acid and diol acidities and the strain release effect. <i>Journal of Physical Organic Chemistry</i> , 0, , . | 0.9 | 3 |
| 16767 | Direct and Water-Mediated Adsorption of Stabilizers on SERS-Active Colloidal Bimetallic Plasmonic Nanomaterials: Insight into Citrate \leftrightarrow AuAg Interactions from DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5236-5251. | 1.1 | 3 |
| 16768 | NHC-catalyzed [3 \rightarrow 4] annulation between 2-dromoenal and aryl 1,2-diamine: Insights into mechanisms, chemo and stereoselectivities. <i>Molecular Catalysis</i> , 2022, 530, 112604. | 1.0 | 1 |
| 16769 | Chemical kinetics of cyclic ethers in combustion. <i>Progress in Energy and Combustion Science</i> , 2022, 92, 101019. | 15.8 | 15 |
| 16770 | An investigation on chain transfer to monomers and initiators, termination of radicals in EVA copolymerization process based on DFT and microkinetic simulation. <i>Polymer</i> , 2022, 256, 125181. | 1.8 | 2 |
| 16771 | Quantum chemical design of near-infrared retinal-based pigments and evaluating their vibronic/electronic properties. <i>Computational and Theoretical Chemistry</i> , 2022, 1215, 113835. | 1.1 | 0 |
| 16772 | Highly efficient removal of organic contaminant with wide concentration range by a novel self-cleaning hydrogel: Mechanism, degradation pathway and DFT calculation. <i>Journal of Hazardous Materials</i> , 2022, 440, 129738. | 6.5 | 14 |
| 16773 | Advances in the development of novel green liquids: thymol/water, thymol/urea and thymol/phenylacetic acid as innovative hydrophobic natural deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2022, 364, 120043. | 2.3 | 10 |
| 16774 | Crystallographic studies of fac- and mer-isomers of Cu[1,4,7,10,13,16-hexaazacyclooctadecane] $_2^{2+}$. Influence of counterion and crystallization solvent on crystal structure and dynamic Jahn-Teller effects. <i>Computational studies of structures, energetics, and mechanism of mer-fac isomerization. Polyhedron</i> , 2022, 225, 116072. | 1.0 | 0 |
| 16775 | Biomimics of [FeFe]-hydrogenases incorporating redox-active ligands: Ferrocene-bridged dithiolate complexes [Fe $_2$ (CO) $_6$ (1 $\frac{1}{4}$ -EC5H4FeC5H4E)] (EA=AS, Se). <i>Journal of Organometallic Chemistry</i> , 2022, 978, 122472. ^{0.8} | | 2 |
| 16776 | Geometric, electronic and spin structures of the CaMn $_4$ O $_5$ catalyst for water oxidation in oxygen-evolving photosystem II. Interplay between experiments and theoretical computations. <i>Coordination Chemistry Reviews</i> , 2022, 471, 214742. | 9.5 | 12 |
| 16777 | Photodegradation of enestroburin in water by simulated sunlight irradiation: Kinetics, isomerization, transformation products identification and toxicity assessment. <i>Science of the Total Environment</i> , 2022, 849, 157725. | 3.9 | 7 |
| 16778 | Thermal decomposition of isopentanol: A theoretical calculation and kinetic modeling analysis. <i>Combustion and Flame</i> , 2022, 245, 112320. | 2.8 | 2 |
| 16779 | Syntheses, Structures, and Biological Activities of Pd(II) and Pt(II) Complexes with some 1-picolinoyl-4-substituted Thiosemicarbazides. <i>Journal of Molecular Structure</i> , 2022, 1269, 133871. | 1.8 | 3 |
| 16780 | A computational investigation about the effect of metal substitutions on the electronic spectra of porphyrin donors in the visible and near infrared regions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 282, 121676. | 2.0 | 1 |
| 16781 | New insight into the mechanism of Pt(0)-catalyzed hydrosilylation reaction of (CH $_3$) $_3$ SiH with CH $_2$ CHSi(CH $_3$) $_3$. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 117, 108294. | 1.3 | 3 |
| 16782 | HOMO-LUMO gaps of large polycyclic aromatic hydrocarbons and their implication on the quantum confinement behavior of flame-formed carbon nanoparticles. <i>Proceedings of the Combustion Institute</i> , 2023, 39, 1069-1077. | 2.4 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16783 | On the formation of C ₅ H ₅ N ⁺ ions in sprayed water microdroplets. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, . | 3.3 | 2 |
| 16784 | Quantum chemical studies on the binding domain of SARS-CoV-2 S-protein: human ACE2 interface complex. Journal of Biomolecular Structure and Dynamics, 2023, 41, 7354-7364. | 2.0 | 1 |
| 16785 | Understanding speciation and solvation of glyphosate from first principles simulations. Journal of Molecular Liquids, 2022, 365, 120154. | 2.3 | 4 |
| 16786 | Assessment of seventeen density functionals to estimate the global reactivity of C20 in the framework of the conceptual density functional theory. Chemical Physics Letters, 2022, 806, 140005. | 1.2 | 1 |
| 16787 | Polymeric organophosphate-hafnium unconventional MOFs nanohybrids enable high-efficiency upgrading of biomass feedstocks via cascade catalytic transfer hydrogenation-dehydration. Industrial Crops and Products, 2022, 188, 115606. | 2.5 | 7 |
| 16788 | Theoretical insight and molecular recognition of oxatub[4]arene-based organic macrocycle as a supramolecular host for antipsychotic drug risperidone. Journal of Molecular Liquids, 2022, 366, 120195. | 2.3 | 2 |
| 16789 | Structure identification of binary (cyclic alcohol guests + methane) clathrate hydrates using Rietveld analysis with the direct space method. Chemical Physics Letters, 2022, 806, 140054. | 1.2 | 7 |
| 16790 | Reconstructing nanofiltration membrane structure and pore size for PA selective layer with different organic solvents based on dissipative particle dynamics. Chemical Engineering Science, 2022, 263, 118096. | 1.9 | 3 |
| 16791 | Making the second generation of molecular motors operate unidirectionally in response to electricity. Materials Today Chemistry, 2022, 26, 101111. | 1.7 | 1 |
| 16792 | Metal-modified s-C3N6 as a potential superior sensing medium for effective capture of toxic waste gases CO, H2S and SO2 in the iron and steel industry based on first-principles investigations. Applied Surface Science, 2022, 606, 154947. | 3.1 | 3 |
| 16793 | Dissolution reaction of TiO2 in molten 6.58NaF-AlF3: A Raman spectroscopy and computational simulation study. Journal of Molecular Liquids, 2022, 367, 120431. | 2.3 | 1 |
| 16794 | Synthesis and properties of AIE-active Triazaborolopyridiniums toward fluorescent nanoparticles for cellular imaging and their biodistribution in vivo and ex vivo. Materials Today Chemistry, 2022, 26, 101121. | 1.7 | 4 |
| 16795 | Redesigning density functional theory with machine learning. , 2023, , 531-558. | | 1 |
| 16796 | Dicyanopyrazino phenanthrene based charge transfer derivatives: Role of amine donor in tuning of photophysical, aggregation-induced emission, electrochemical and theoretical properties. Journal of Molecular Structure, 2023, 1271, 134052. | 1.8 | 3 |
| 16797 | Density-functional theory. , 2023, , 27-65. | | 0 |
| 16798 | Synthesis of new sulfamate linked 4-hydroxycoumarin conjugates as potent anti- α -amylase agents: In vitro approach coupled with molecular docking, DFT calculation and chemoinformatics prediction. Journal of Molecular Structure, 2023, 1271, 134020. | 1.8 | 5 |
| 16799 | Influence of <i>N</i> - and <i>P</i> -substituents in <i>N</i> -aryl-phosphinoglycine ligands on the selectivity of Ni-catalysed ethylene oligomerization. New Journal of Chemistry, 2022, 46, 17303-17312. | 1.4 | 2 |
| 16800 | Molecular recognition and spectral tuning of organic dyes in water by amide naphthotubes. Chemical Communications, 2022, 58, 9413-9416. | 2.2 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16801 | Deciphering the Cooperative Effect of Base and N-Substituents on the Origin of Regioselectivity Switching for Mannich Reactions of Glycinate by Carbonyl Catalysts. SSRN Electronic Journal, 0, , . | 0.4 | 0 |
| 16802 | Interaction between glyphosate pesticide and amphiphilic peptides for colorimetric analysis. Nanoscale Advances, 2022, 4, 3592-3599. | 2.2 | 1 |
| 16803 | Iron L ₃ -edge energy shifts for the full range of possible 3d occupations within the same oxidation state of iron halides. Physical Chemistry Chemical Physics, 2022, 24, 19890-19894. | 1.3 | 5 |
| 16804 | Simulation and analysis of the relaxation dynamics of a photochromic furylfulgide. Physical Chemistry Chemical Physics, 2022, 24, 18103-18118. | 1.3 | 4 |
| 16805 | DFT studies on rhodium(ⁱⁱⁱ)-catalyzed synthesis of indanones from <i>N</i> -methoxybenzamides <i>via</i> C-H activation reaction. New Journal of Chemistry, 2022, 46, 16576-16583. | 1.4 | 0 |
| 16806 | The annulation of <i>N</i> -hydroxyoximes and 1,3-diyne to synthesize alkynylated isoquinolines regioselectively catalyzed by ruthenium: a theoretical study. Organic and Biomolecular Chemistry, 2022, 20, 7294-7301. | 1.5 | 2 |
| 16807 | Pericyclic reaction benchmarks: hierarchical computations targeting CCSDT(Q)/CBS and analysis of DFT performance. Physical Chemistry Chemical Physics, 2022, 24, 18028-18042. | 1.3 | 14 |
| 16808 | Side Chain effect on the electrochemical and optical properties of thieno[3,4- <i>c</i>]pyrrole-4,6-dione based donor acceptor donor type monomers and polymers. Molecular Systems Design and Engineering, 0, , . | 1.7 | 3 |
| 16809 | Evaluating fast methods for static polarizabilities on extended conjugated oligomers. Physical Chemistry Chemical Physics, 2022, 24, 23173-23181. | 1.3 | 1 |
| 16810 | Roadmap for point defects in GaN. Semiconductors and Semimetals, 2022, , . | 0.4 | 0 |
| 16811 | Concerted addition of aldehydes to the singlet biradical [P(¹ / ₄ -Nter)] ₂ . Dalton Transactions, 2022, 51, 13479-13487. | 1.6 | 2 |
| 16812 | Density Functional Theory on the CO ₂ Absorption Process with Ionic Liquids. Computer Aided Chemical Engineering, 2022, , 967-972. | 0.3 | 0 |
| 16813 | A theoretical study on the donor ability adjustment of tris(2,4,6-trichlorophenyl)methyl-triarylamine (TTM-TPA) radicals aiming to develop better organic luminescent materials. New Journal of Chemistry, 2022, 46, 16325-16332. | 1.4 | 5 |
| 16814 | Comprehending radicals, diradicals and their bondings in aggregates of imide-fused polycyclic aromatic hydrocarbons. Chemical Science, 2022, 13, 9985-9992. | 3.7 | 2 |
| 16815 | Fluoride Transport and Inhibition Across CLC Transporters. Handbook of Experimental Pharmacology, 2022, , 81-100. | 0.9 | 0 |
| 16816 | The role of the intermediate triplet state in iron-catalyzed multi-state C-H activation. Physical Chemistry Chemical Physics, 2022, 24, 20721-20727. | 1.3 | 1 |
| 16817 | Evaluating the impact of Hartree-Fock exact exchange on the performance of global hybrid functionals for the vertical excited-state energies of fused-ring electron acceptors using TD-DFT. Physical Chemistry Chemical Physics, 2022, 24, 21270-21282. | 1.3 | 1 |
| 16818 | Network metrics, structural dynamics and density functional theory calculations identified a novel Ursodeoxycholic Acid derivative against therapeutic target Parkin for Parkinson's disease. Computational and Structural Biotechnology Journal, 2022, 20, 4271-4287. | 1.9 | 18 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16819 | Ruthenium phthalocyanines in nitric oxide modulation and singlet oxygen release: Selectivity and cytotoxic effect on cancer cell lines. <i>Advances in Inorganic Chemistry</i> , 2022, , . | 0.4 | 2 |
| 16820 | Unveiling the structure of aqueous magnesium nitrate solutions by combining X-ray diffraction and theoretical calculations. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 22939-22949. | 1.3 | 4 |
| 16821 | Ni(η^5 -TPA) stabilization by hydrogen bond formation on the second coordination sphere: a DFT characterization. <i>Dalton Transactions</i> , 2022, 51, 12585-12595. | 1.6 | 3 |
| 16822 | The smallest 4f-metalla-aromatic molecule of cyclo-PrB ₂ ⁺ with Pr π -B multiple bonds. <i>Chemical Science</i> , 2022, 13, 10082-10094. | 3.7 | 4 |
| 16823 | Vibrational Spectroscopic Investigations, Electronic Properties, Molecular Structure and Quantum Mechanical Study of an Antifolate Drug: Pyrimethamine. <i>Computational Chemistry</i> , 2022, 10, 157-185. | 0.2 | 2 |
| 16824 | Facile supramolecular strategy to construct solid fluorophore@metal-organic framework composites. <i>Materials Advances</i> , 2022, 3, 6597-6608. | 2.6 | 0 |
| 16825 | A Theoretical Investigation of the Possible Mechanisms for Detection the Copper Ions by a Retinal-Base Sensor. <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 0 |
| 16826 | The S ⁺ +SiH ₂ Reaction: Toward the Synthesis of Interstellar SiS. <i>Lecture Notes in Computer Science</i> , 2022, , 233-245. | 1.0 | 1 |
| 16827 | Heterodimetallic Iridium-Rhenium System: Synthesis, Computational and Photocatalytic Aspects. <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 0 |
| 16828 | Fragmentation of interstellar methanol by collisions with He ⁺ : an experimental and computational study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 22437-22452. | 1.3 | 5 |
| 16829 | Computational thermochemistry: extension of Benson group additivity approach to organoboron compounds and reliable predictions of their thermochemical properties. <i>Dalton Transactions</i> , 0, , . | 1.6 | 0 |
| 16830 | How reduced are nucleophilic gold complexes?. <i>Dalton Transactions</i> , 2022, 52, 11-15. | 1.6 | 7 |
| 16831 | Non-Aufbau orbital ordering and spin density modulation in high-spin donor-acceptor conjugated polymers. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 23699-23711. | 1.3 | 4 |
| 16832 | Inverse potential scaling in co-electrocatalytic activity for CO ₂ reduction through redox mediator tuning and catalyst design. <i>Chemical Science</i> , 2022, 13, 9595-9606. | 3.7 | 6 |
| 16833 | Cr/PCCP-catalysed selective ethylene oligomerization: analysis of various conformations and the hemilabile methoxy group. <i>Catalysis Science and Technology</i> , 2022, 12, 5586-5596. | 2.1 | 10 |
| 16834 | π -Orbital mediated charge transfer channels in a monolayer Gr π -NiPc heterointerface unveiled by soft X-ray electron spectroscopies and DFT calculations. <i>Nanoscale</i> , 2022, 14, 13166-13177. | 2.8 | 2 |
| 16835 | The effect of particle size and composition on the optical and electronic properties of CdO and CdS rocksalt nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 21954-21965. | 1.3 | 0 |
| 16836 | DFT exchange: sharing perspectives on the workhorse of quantum chemistry and materials science. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 28700-28781. | 1.3 | 91 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16837 | Studies of a bola-type bis(dithiafulvene) molecular system: synthesis, crystal structure, and electrochemical properties. <i>New Journal of Chemistry</i> , 2022, 46, 18133-18145. | 1.4 | 1 |
| 16838 | Resolving the σ -assisted $U\text{-}N$ σ -bond formation using quantum information theory. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 21296-21307. | 1.3 | 5 |
| 16839 | Reaction dynamics of Diels-Alder reactions from machine learned potentials. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20820-20827. | 1.3 | 8 |
| 16840 | Dft Computational Study of Optical Properties for Bis-Schiff Bases of 8-Aminoquinoline Derivatives and Furan-2, 3-Di-Carbaldehyd. <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 1 |
| 16841 | Study on the effect of solvent on cocrystallization of CL-20 and HMX through theoretical calculations and experiments. <i>RSC Advances</i> , 2022, 12, 21255-21263. | 1.7 | 0 |
| 16842 | Induction and rationalization of supramolecular chirality in a highly flexible Zn(<i>ii</i>)porphyrin dimer: structural, spectroscopic and theoretical investigations. <i>Dalton Transactions</i> , 2022, 51, 14125-14137. | 1.6 | 1 |
| 16843 | Tuning the anticancer properties of Pt(<i>ii</i>) complexes <i>via</i> structurally flexible N -(2-picolyl)salicylimine ligands. <i>RSC Advances</i> , 2022, 12, 27582-27595. | 1.7 | 6 |
| 16844 | Linear conjugated polymer photocatalysts with various linker units for photocatalytic hydrogen evolution from water. <i>Chemical Communications</i> , 2022, 58, 10639-10642. | 2.2 | 6 |
| 16845 | Effect of conformational disorder on exciton states of an azobenzene aggregate. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 24002-24006. | 1.3 | 3 |
| 16846 | Vanadium pyridonates: dimerization, redox behaviour, and metal-ligand cooperativity. <i>Dalton Transactions</i> , 2022, 51, 14654-14663. | 1.6 | 2 |
| 16847 | Theoretical investigations on the antioxidant potential of 2,4,5-trihydroxybutyrophenone in different solvents: A DFT approach. <i>Results in Chemistry</i> , 2022, 4, 100515. | 0.9 | 4 |
| 16848 | A Theoretical Investigation of the Reactions of N_2 and HCN with Acrylonitrile and Implications for Prebiotic Chemistry of Titan. <i>Lecture Notes in Computer Science</i> , 2022, , 246-259. | 1.0 | 0 |
| 16849 | Probing the effect of microenvironment on the enzyme-like behavior of catalytic peptide assemblies. <i>Journal of Colloid and Interface Science</i> , 2023, 629, 683-693. | 5.0 | 3 |
| 16850 | Efficient removal of polybrominated diphenyl ethers from soil washing effluent by dummy molecular imprinted adsorbents: Selectivity and mechanisms. <i>Journal of Environmental Sciences</i> , 2023, 129, 45-57. | 3.2 | 7 |
| 16851 | Thermally Induced Solid-Phase Quasi-Intramolecular Redox Reactions of [Hexakis(urea- O)iron(III)] Permanganate: An Easy Reaction Route to Prepare Potential (Fe,Mn) O_x Catalysts for CO_2 Hydrogenation. <i>Inorganic Chemistry</i> , 2022, 61, 14403-14418. | 1.9 | 9 |
| 16852 | Reproducibility of Hybrid Density Functional Calculations for Equation-of-State Properties and Band Gaps. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5924-5931. | 1.1 | 7 |
| 16853 | Controlling Interfacial Structural Evolution in Aqueous Electrolyte via Anti-Electrolytic Zwitterionic Waterproofing. <i>Advanced Functional Materials</i> , 2022, 32, . | 7.8 | 7 |
| 16854 | Rational design, synthesis, and pharmacological characterisation of dicarbonyl curcuminoid analogues with improved stability against lung cancer via ROS and ER stress mediated cell apoptosis and pyroptosis. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2022, 37, 2357-2369. | 2.5 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16855 | Comparative Analysis of Interaction Mode between MABA and Silver Nanoparticles in the Silver Colloidal Solution. Russian Journal of Physical Chemistry B, 2022, 16, 590-595. | 0.2 | 0 |
| 16856 | Microbial biofilms as living photoconductors due to ultrafast electron transfer in cytochrome OmcS nanowires. Nature Communications, 2022, 13, . | 5.8 | 24 |
| 16857 | What It Takes for Imidazolium Cations to Promote Electrochemical Reduction of CO ₂ . ACS Energy Letters, 2022, 7, 3439-3446. | 8.8 | 12 |
| 16858 | Parametrization of the PM7 Semiempirical Quantum Mechanical Method for Silver Nanoclusters. Journal of Physical Chemistry A, 2022, 126, 6558-6569. | 1.1 | 0 |
| 16859 | Comprehensive evaluation of end-point free energy techniques in carboxylated-pillar[6]arene host-guest binding: I. Standard procedure. Journal of Computer-Aided Molecular Design, 2022, 36, 735-752. | 1.3 | 7 |
| 16860 | Accurate Vertical Excitation Energies of BODIPY/Aza-BODIPY Derivatives from Excited-State Mean-Field Calculations. Journal of Physical Chemistry A, 0, , . | 1.1 | 5 |
| 16861 | Electronic and Vibrational Manifold of Tetracyanoethylene-Chloronaphthalene Charge Transfer Complex in Solution: Insights from TD-DFT and Ab Initio Molecular Dynamics. Journal of Physical Chemistry A, 2022, 126, 7179-7192. | 1.1 | 5 |
| 16862 | Antioxidant and anticancer properties of plant-based bioactive flavonoids cardamomin and alpinetin: A theoretical insight from ⁰⁰ OOH antiradical and Cu (II) chelation mechanisms. Journal of Physical Organic Chemistry, 0, , . | 0.9 | 2 |
| 16863 | Chemical bonding between thorium and novel BN nanomaterials. Journal of Applied Physics, 2022, 132, 124302. | 1.1 | 0 |
| 16864 | Combining molecular modeling approaches to establish the chromatographic enantiomer elution order in the absence of pure enantiomeric standards: A study case with two tetracyclic quinolines. Separation Science Plus, 2022, 5, 662-670. | 0.3 | 2 |
| 16865 | Theoretical study of the interaction of fullerenes with the emerging contaminant carbamazepine for detection in aqueous environments. Scientific Reports, 2022, 12, . | 1.6 | 6 |
| 16866 | Chemosensing Properties of Coumarin Derivatives: Promising Agents with Diverse Pharmacological Properties, Docking and DFT Investigation. Molecules, 2022, 27, 5921. | 1.7 | 6 |
| 16867 | The performance of exchange-correlation functionals in describing electron density parameters of saddle point structures along chemical reactions. Journal of Computational Chemistry, 2022, 43, 1830-1838. | 1.5 | 1 |
| 16868 | Electronic structure of O_3 grain boundaries containing reactive element segregants. Physical Review Materials, 2022, 6, . | 0.9 | 1 |
| 16869 | Reaction N(² D) + CH ₂ CCH ₂ (Allene): An Experimental and Theoretical Investigation and Implications for the Photochemical Models of Titan. ACS Earth and Space Chemistry, 2022, 6, 2305-2321. | 1.2 | 6 |
| 16870 | Theoretical study on a series of naphthalimide-contained two-photon fluorescent hypochlorite probe targeting endoplasmic reticulum: response mechanism and receptor effect. Journal of Molecular Modeling, 2022, 28, . | 0.8 | 0 |
| 16871 | Benchmark of density functional theory methods for the study of organic polysulfides. Journal of Computational Chemistry, 2022, 43, 2131-2138. | 1.5 | 6 |
| 16872 | Static Electron Correlation in Anharmonic Molecular Vibrations: A Hybrid TAO-DFT Study. Journal of Physical Chemistry A, 2022, 126, 7273-7282. | 1.1 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 16873 | Interaction between the Human OX2 Orexin Receptor and Suvorexant and Some of Its Analogues: SAPT (DFT) Interaction Energy Decomposition Analysis. <i>Journal of Physical Chemistry B</i> , 2022, 126, 7528-7540. | 1.2 | 0 |
| 16874 | Tertiary and Quaternary Phosphonium Borane Bifunctional Catalysts for CO ₂ /Epoxide Copolymerization: A Mechanistic Investigation Using In Situ Raman Spectroscopy. <i>ACS Catalysis</i> , 2022, 12, 11870-11885. | 5.5 | 18 |
| 16875 | Modeling pK _a of the Brønsted Bases as an Approach to the Gibbs Energy of the Proton in Acetonitrile. <i>International Journal of Molecular Sciences</i> , 2022, 23, 10576. | 1.8 | 4 |
| 16876 | Application of catalysts in the synthesis of 4-(4-(dimethylamino)benzylidene)-3-methylisoxazol-5(4H)-one: experimental and theoretical studies. <i>Applied Physics A: Materials Science and Processing</i> , 2022, 128, . | 1.1 | 1 |
| 16877 | Design of Smart Aggregates: Toward Rapid Clinical Diagnosis of Hyperlipidemia in Human Blood. <i>Advanced Materials</i> , 2022, 34, . | 11.1 | 12 |
| 16878 | The N ² + CH ₂ CHCN (Vinyl Cyanide) Reaction: A Combined Crossed Molecular Beam and Theoretical Study and Implications for the Atmosphere of Titan. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6110-6123. | 1.1 | 10 |
| 16879 | Accurate pK _a Calculations in Proteins with Reactive Molecular Dynamics Provide Physical Insight Into the Electrostatic Origins of Their Values. <i>Journal of Physical Chemistry B</i> , 2022, 126, 7321-7330. | 1.2 | 2 |
| 16880 | Multiconfigurational short-range density functional theory for nuclear magnetic resonance shielding constants with gauge-including atomic orbitals. <i>Journal of Chemical Physics</i> , 0, . | 1.2 | 1 |
| 16881 | Density functionals for core excitations. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 1 |
| 16882 | Probing Isomerization Dynamics via a Dipole-Bound State. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 8711-8716. | 2.1 | 1 |
| 16883 | Cheap Turns Superior: A Linear Regression-Based Correction Method to Reaction Energy from the DFT. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 4727-4735. | 2.5 | 1 |
| 16884 | In the quest of H ₄ Ckel and H ₄ Ckel Baird double aromatic tropylium (tri)cation and anion derivatives. <i>Journal of Physical Organic Chemistry</i> , 0, . | 0.9 | 3 |
| 16885 | Promoting Catalytic Activity of Boron by Phosphor in Propane Oxidative Dehydrogenation. <i>Journal of Physical Chemistry C</i> , 2022, 126, 16672-16681. | 1.5 | 2 |
| 16886 | Singlet Fission from Upper Excited States of Bodipy Crystalline Film and Single Crystal. <i>Journal of Physical Chemistry C</i> , 2022, 126, 17212-17222. | 1.5 | 3 |
| 16887 | Synthesis of Amide Enol 2-Iodobenzoates by the Regio- and Stereoselective Gold-Catalyzed Acyloxyalkynylation of Ynamides with Hypervalent Iodine Reagents. <i>Organic Letters</i> , 2022, 24, 7101-7106. | 2.4 | 13 |
| 16888 | Best Practice DFT Protocols for Basic Molecular Computational Chemistry**. <i>Angewandte Chemie</i> , 2022, 134, . | 1.6 | 36 |
| 16889 | Charge Transfer Transitions Govern the Reactivity and Photophysics of Vicinally Diphosphanyl-Substituted Diborapentacenes. <i>Chemistry - A European Journal</i> , 0, . | 1.7 | 6 |
| 16890 | Cyclometalated Spirofluorene Imidazolylidene Platinum(II) Complexes with Predominant ³ LC Emissive Character and High Photoluminescence Quantum Yields. <i>Inorganic Chemistry</i> , 2022, 61, 15499-15509. | 1.9 | 4 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16891 | Cost-Effective Implementation of Multiconformer Transition State Theory for Alkoxy Radical Unimolecular Reactions. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6483-6494. | 1.1 | 4 |
| 16892 | Halogenated Carboxylates as Organic Anodes for Stable and Sustainable Sodium-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 40784-40792. | 4.0 | 11 |
| 16893 | Best Practice DFT Protocols for Basic Molecular Computational Chemistry**. <i>Angewandte Chemie - International Edition</i> , 2022, 61, . | 7.2 | 168 |
| 16894 | Comprehensive Approach to the Interpretation of the Electrical Properties of Film-Forming Molecules. <i>Journal of Physical Chemistry B</i> , 2022, 126, 7037-7046. | 1.2 | 3 |
| 16895 | Rational Molecular Design Enables Efficient Blue TADF ^o OLEDs with Flexible Graphene Substrate. <i>Advanced Functional Materials</i> , 2022, 32, . | 7.8 | 15 |
| 16896 | Quantitative Structure-Property Relationship Model for Predicting the Propagation Rate Coefficient in Free-Radical Polymerization. <i>Macromolecules</i> , 2022, 55, 9397-9410. | 2.2 | 12 |
| 16897 | Revisiting the pyrolysis of 1,5-diaryla-1,2,5-triazapentadienes: A computational reaction mechanism study. <i>ChemistrySelect</i> , 2022, 7, . | 0.7 | 0 |
| 16898 | Can armchair nanotubes host organic color centers?. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 464004. | 0.7 | 0 |
| 16899 | Electronic Structures and Unusual Chemical Bonding in Actinyl Peroxide Dimers [An ₂ O ₆] ²⁺ and [(An ₂ O ₆)(12-crown-4)] ⁺ . <i>Journal of Physical Chemistry A</i> , 2022, 126, 7013-7020. | 1.1 | 3 |
| 16900 | Unusual Enantiodivergence in Chiral Brønsted Acid-Catalyzed Asymmetric Allylation with ² Alkenyl Allylic Boronates. <i>Angewandte Chemie - International Edition</i> , 2022, 61, . | 7.2 | 9 |
| 16901 | The four-component DFT method for the calculation of the EPR g-tensor using a restricted magnetically balanced basis and London atomic orbitals. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 2 |
| 16902 | Metal-Catalyzed Formation of Organic Pollutants Intermediated by Organic Free Radicals. <i>Environmental Science & Technology</i> , 2022, 56, 14550-14561. | 4.6 | 4 |
| 16903 | Vibrational Corrections to NMR Spin-Spin Coupling Constants from Relativistic Four-Component DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7013-7020. | 1.1 | 3 |
| 16904 | Cytotoxic mixed-ligand complexes of Cu(II): A combined experimental and computational study. <i>Frontiers in Chemistry</i> , 0, 10, . | 1.8 | 6 |
| 16905 | Facile Synthesis of Liquid Crystal Dimers Bridged with a Phosphonic Group. <i>Chemistry - A European Journal</i> , 2022, 28, . | 1.7 | 6 |
| 16906 | Efficient Copper-Catalyzed Highly Stereoselective Synthesis of Unprotected C ₆ -Acyl Manno ^o , Rhamno ^o and Lyxopyranosides. <i>Chemistry - A European Journal</i> , 0, , . | 1.7 | 1 |
| 16907 | LIDA: The Leiden Ice Database for Astrochemistry. <i>Astronomy and Astrophysics</i> , 2022, 668, A63. | 2.1 | 11 |
| 16908 | 4-component relativistic Hamiltonian with effective QED potentials for molecular calculations. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 17 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16909 | Multiple resonance type thermally activated delayed fluorescence by dibenzo [1,4] azaborine derivatives. <i>Frontiers in Chemistry</i> , 0, 10, . | 1.8 | 7 |
| 16910 | Computational investigation of the aza-Cope rearrangement leading to angularly substituted 1-azabicyclic rings. <i>Synlett</i> , 0, , . | 1.0 | 0 |
| 16911 | Critical analysis of radical scavenging properties of atorvastatin in methanol recently estimated via density functional theory. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113898. | 1.1 | 3 |
| 16912 | Polyamide composite membranes for enhanced organic solvent nanofiltration performance by metal ions assisted interfacial polymerization method. <i>AIChE Journal</i> , 2023, 69, . | 1.8 | 7 |
| 16913 | Aziridination Reactivity of a Manganese(II) Complex with a Bulky Chelating Bis(Alkoxide) Ligand. <i>Molecules</i> , 2022, 27, 5751. | 1.7 | 0 |
| 16914 | From Gas Phase Observations to Solid State Reality: The Identification and Isolation of Trinuclear Salicylaldoximate Copper Complexes. <i>Molecules</i> , 2022, 27, 6421. | 1.7 | 0 |
| 16915 | Computational Studies Followed by Effect of Solvent Polarity and Salts on HOMO–LUMO Gap of 7-Hydroxy Coumarine Notably Reflected by Absorption and Emission Spectra. <i>Journal of Fluorescence</i> , 2022, 32, 2351-2362. | 1.3 | 3 |
| 16916 | CuI COMPLEXES BASED ON DI(2-PYRIDYL) (2-ARYLETHENYL)PHOSPHINE OXIDES: SYNTHESIS, STRUCTURE, AND DARK RED PHOTOLUMINESCENCE. <i>Journal of Structural Chemistry</i> , 2022, 63, 1383-1389. | 0.3 | 1 |
| 16917 | A computational approach for modeling electronic circular dichroism of solvated chromophores. <i>Journal of Computational Chemistry</i> , 2022, 43, 2023-2036. | 1.5 | 10 |
| 16918 | Metal–Support Interactions in Molecular Single-Site Cluster Catalysts. <i>Journal of the American Chemical Society</i> , 2022, 144, 18459-18469. | 6.6 | 8 |
| 16919 | Filling the Gaps in the Challenging Asymmetric Hydrogenation of Exocyclic Benzofused Alkenes with Ir ^{III} P,N Catalysts. <i>Advanced Synthesis and Catalysis</i> , 2023, 365, 167-177. | 2.1 | 4 |
| 16920 | Theoretical insights on alleviating lattice-oxygen evolution by sulfur substitution in Li _{1.2} Ni _{0.6} Mn _{0.2} O ₂ cathode material. <i>Npj Computational Materials</i> , 2022, 8, . | 3.5 | 5 |
| 16921 | ¹³ C ENDOR Characterization of the Central Carbon within the Nitrogenase Catalytic Cofactor Indicates That the CFe ₆ Core Is a Stabilizing “Heart of Steel”. <i>Journal of the American Chemical Society</i> , 2022, 144, 18315-18328. | 6.6 | 11 |
| 16922 | Probing Intermolecular H-Bonding Interactions in Cyanuric Acid Networks: Quenching of the N-Edge Sigma Resonances. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6870-6881. | 1.1 | 2 |
| 16923 | Interactions of Curcumin’s Degradation Products with the Al ₂ Dimer: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2022, 126, 7627-7637. | 1.2 | 4 |
| 16924 | Effect of Protonation and Deprotonation on Electron Transfer Mediated Decay and Interatomic Coulombic Decay. <i>ChemPhysChem</i> , 0, , . | 1.0 | 1 |
| 16925 | Optimization of density fitting auxiliary Slater-type basis functions for time-dependent density functional theory. <i>Journal of Computational Chemistry</i> , 2022, 43, 1923-1935. | 1.5 | 5 |
| 16926 | Cherry-Picking Resolvents: Recovering the Valence Contribution in X-ray Two-Photon Absorption within the Core–Valence-Separated Equation-of-Motion Coupled-Cluster Response Theory. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 6189-6202. | 2.3 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16927 | Transient Absorption Spectroscopy of a Carbazole-Based Room-Temperature Phosphorescent Molecule: Real-Time Monitoring of Singlet-Triplet Transitions. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 9381-9389. | 2.1 | 14 |
| 16928 | Gold-Catalyzed Bidirectional Access to Planar Heptacyclic Benzobispyrido[1,2-a]indoles and Benzobispyrrolo[1,2-a]Quinolines for Materials Science. <i>Advanced Synthesis and Catalysis</i> , 2022, 364, 3559-3566. | 2.1 | 3 |
| 16929 | Rapid calculation of internal conversion and intersystem crossing rate for organic materials discovery. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 5 |
| 16930 | Charge Delocalization and Vibronic Couplings in Quadrupolar Squaraine Dyes. <i>Journal of the American Chemical Society</i> , 2022, 144, 19150-19162. | 6.6 | 7 |
| 16931 | Probabilistic Interpretation of NMR J -Couplings Determines Blå“BII State Equilibria in DNA. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 6989-6999. | 2.3 | 2 |
| 16932 | A Solid/Liquid High-Energy-Density Storage Concept for Redox Flow Batteries and Its Demonstration in an H_2 - V System. <i>Journal of the Electrochemical Society</i> , 2022, 169, 110509. | 1.3 | 3 |
| 16933 | Highly Sensitive Zwitterionic Hydrogel Sensor for Motion and Pulse Detection with Water Retention, Adhesive, Antifreezing, and Self-Healing Properties. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 47100-47112. | 4.0 | 24 |
| 16934 | High-temperature mid-IR absorption spectra and reaction kinetics of 1,3-dioxolane. <i>Proceedings of the Combustion Institute</i> , 2023, 39, 621-631. | 2.4 | 4 |
| 16935 | Wavefunction frozen-density embedding with one-dimensional periodicity: Electronic polarization effects from local perturbations. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 1 |
| 16936 | Development of a novel ReaxFF reactive potential for organochloride molecules. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 1 |
| 16937 | Mononuclear manganese complexes as hydrogen evolving catalysts. <i>Frontiers in Chemistry</i> , 0, 10, . | 1.8 | 1 |
| 16938 | New isoflavan from <i>Erythrina livingstoniana</i> . <i>Natural Product Research</i> , 2024, 38, 493-502. | 1.0 | 0 |
| 16940 | How good are recent density functionals for ground and excited states of one-electron systems?. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 6 |
| 16941 | Molecular-based asphalt oxidation reaction mechanism and aging resistance optimization strategies based on quantum chemistry. <i>Materials and Design</i> , 2022, 223, 111225. | 3.3 | 11 |
| 16942 | Noncovalent minimal assembly of exogenous histamine with hemin cofactor as a peroxidase-mimicking cooperative catalyst. <i>IScience</i> , 2022, 25, 105257. | 1.9 | 2 |
| 16943 | Mechanistic Study on Palladium-Catalyzed Cycloaddition of Vinyl-ethylene Carbonates with β,γ -Unsaturated Imines. <i>Organometallics</i> , 2022, 41, 2844-2853. | 1.1 | 1 |
| 16944 | Sensitivity of coupled cluster electronic properties on the reference determinant: Can Kohn-Sham orbitals be more beneficial than Hartree-Fock orbitals?. <i>Journal of Computational Chemistry</i> , 0, , . | 1.5 | 4 |
| 16945 | Unusual pathway of epoxide hydration over a novel CoIII(salen)-based pseudohomogeneous catalyst with excellent performance. <i>Journal of Catalysis</i> , 2022, 414, 365-373. | 3.1 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 16946 | Wide-range IR spectra of diarylethene derivatives and their simulation using the density functional theory. <i>Scientific Reports</i> , 2022, 12, . | 1.6 | 1 |
| 16947 | Deciphering the cooperative effect of base and N-substituents on the origin of enantioselectivity switching for Mannich reactions of glycinate by carbonyl catalysts. <i>Journal of Catalysis</i> , 2022, 415, 1-11. | 3.1 | 4 |
| 16948 | An efficient initiator system containing AlCl ₃ and supported ionic-liquid for the synthesis of conventional grade polyisobutylene in mild conditions. <i>Journal of Molecular Liquids</i> , 2022, 367, 120381. | 2.3 | 12 |
| 16949 | Molecular modelling of ionic liquids: Physical properties of species with extremely long aliphatic chains from a near-optimal regime. <i>Journal of Molecular Liquids</i> , 2022, 367, 120492. | 2.3 | 9 |
| 16950 | Photoredox catalysis leading to triazolo-quinoxalinones at room temperature: selectivity of the rate determining step. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 9330-9336. | 1.5 | 3 |
| 16951 | Synthesis and characterization of CuO@S-doped g-C ₃ N ₄ based nanocomposites for binder-free sensor applications. <i>RSC Advances</i> , 2022, 12, 29959-29974. | 1.7 | 9 |
| 16952 | Structure determination and bonding properties of gas-phase OPt ₂ ⁺ anion and its neutral form. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 26023-26028. | 1.3 | 1 |
| 16953 | Versatile access to nitrogen-rich π -extended indolocarbazoles via a Pictet-Spengler approach. <i>Organic Chemistry Frontiers</i> , 2022, 10, 12-21. | 2.3 | 3 |
| 16954 | Ru/Rh catalyzed selective hydrogenation of CO ₂ to formic acid: a first principles microkinetics analysis. <i>Catalysis Science and Technology</i> , 2022, 12, 7219-7232. | 2.1 | 7 |
| 16955 | Facilitating <i>ab initio</i> QM/MM free energy simulations by Gaussian process regression with derivative observations. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 25134-25143. | 1.3 | 7 |
| 16956 | DFT Calculations for Structural, Electronic, and Magnetic Properties of ZnFe ₂ O ₄ Spinel Oxide: The Role of Exchange-Correlation Functional. <i>Materials Research</i> , 0, 25, . | 0.6 | 4 |
| 16957 | Hydrogen bond networks in gas-phase complex anions. <i>RSC Advances</i> , 2022, 12, 29137-29142. | 1.7 | 0 |
| 16958 | The effect of halides and coordination mode of 4-amino-2,1,3-benzothiadiazole on the luminescence properties of its Zn complexes. <i>CrystEngComm</i> , 2022, 24, 8256-8265. | 1.3 | 2 |
| 16959 | Impact of molecular chain length on polarizabilities of model acenes and oligomers. <i>Acta Chimica Slovaca</i> , 2022, 15, 117-122. | 0.5 | 0 |
| 16960 | Mechanism of [3+2] Annulations between Indole-2-formaldehydes and Isatins Mediated by N-Heterocyclic Carbene: A DFT Study. <i>New Journal of Chemistry</i> , 0, , . | 1.4 | 0 |
| 16961 | Curcumin-based ionic Pt(II) complexes: antioxidant and antimicrobial activity. <i>Dalton Transactions</i> , 2022, 51, 16545-16556. | 1.6 | 2 |
| 16962 | Which DFT factors influence the accuracy of ¹ H, ¹³ C and ¹⁹⁵ Pt NMR chemical shift predictions in organopolymetallic square-planar complexes? New scaling parameters for homo- and hetero-multimetallic compounds and their direct applications. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 26642-26658. | 1.3 | 6 |
| 16963 | Modulation of the magnetic dynamics of pentagonal-bipyramidal Co(II) complexes by fine-tuning the coordination microenvironment. <i>Dalton Transactions</i> , 2022, 51, 17089-17096. | 1.6 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 16964 | The activated reaction of dichlorocarbene with triplet molecular oxygen. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 25834-25841. | 1.3 | 0 |
| 16965 | Thermodynamics of self-assembled molecular layers of trimesic acid from fields-supported kinetic Monte Carlo simulation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 26111-26123. | 1.3 | 4 |
| 16966 | Organocatalytic enantioselective synthesis of dihydronaphthofurans and dihydrobenzofurans: reaction development and insights into stereoselectivity. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 8725-8740. | 1.5 | 1 |
| 16967 | Enhancement of DNAzymatic activity using iterative <i>in silico</i> maturation. <i>Journal of Materials Chemistry B</i> , 0, , . | 2.9 | 0 |
| 16968 | A polarizable coarse-grained model for metal, metal oxide and composite metal/metal oxide nanoparticles and its applications. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 27742-27750. | 1.3 | 1 |
| 16969 | Theoretical study on the structures, electronic properties, and aromaticity of thia[4]circulenes. <i>New Journal of Chemistry</i> , 2022, 46, 22703-22714. | 1.4 | 3 |
| 16970 | Spectral properties of Ni(II) complex of a tridentate pyridine-amide ligand with appended ether functionality [n-(2-Methoxyphenyl)picolinamide]: Theoretical and Experimental studies. <i>Journal of Physics: Conference Series</i> , 2022, 2349, 012023. | 0.3 | 0 |
| 16971 | Microwave spectra of two conformers of the (1R)-(â€‘)-nopol monomer. <i>Journal of Molecular Spectroscopy</i> , 2022, 389, 111705. | 0.4 | 1 |
| 16972 | A computational study of the inclusion of β -cyclodextrin and nicotinic acid: DFT, DFT-D, NPA, NBO, QTAIM, and NCI-RDG studies. <i>Journal of Molecular Modeling</i> , 2022, 28, . | 0.8 | 6 |
| 16973 | A Carboxylic Ester-Based Electrolyte with Additive to Improve Performance of Lithium Batteries at Ultra-Low Temperature. <i>Journal of the Electrochemical Society</i> , 2022, 169, 100539. | 1.3 | 3 |
| 16974 | Antibacterial and Antioxidant Activities, <i>in silico</i> Molecular Docking, ADMET and DFT Analysis of Compounds from Roots of <i>Cyphostemma cyphopetalum</i> . <i>Advances and Applications in Bioinformatics and Chemistry</i> , 0, Volume 15, 79-97. | 1.6 | 2 |
| 16975 | On the Role of Noncovalent Ligand-Substrate Interactions in Au(I) Catalysis: An Experimental and Computational Study of Protodeauration. <i>ACS Catalysis</i> , 2022, 12, 13158-13163. | 5.5 | 4 |
| 16976 | The Bonding Nature of Feâ€‘CO Complexes in Heme Proteins. <i>Inorganic Chemistry</i> , 2022, 61, 17494-17504. | 1.9 | 5 |
| 16977 | Chemical bonding in representative astrophysically relevant neutral, cation, and anion HC _n chains. <i>Chinese Physics B</i> , 2022, 31, 123101. | 0.7 | 2 |
| 16978 | New Insight into CO ₂ Reduction to Formate by In Situ Hydrogen Produced from Hydrothermal Reactions with Iron. <i>Molecules</i> , 2022, 27, 7371. | 1.7 | 2 |
| 16980 | Thermodynamics of the Metal Carbonates and Bicarbonates of Mn, Co, Ni, Cu, and Zn Relevant to Mineral Energetics. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7874-7887. | 1.1 | 2 |
| 16981 | 3â€‘-Aminothiocylohexanespiro-5â€‘-hydantoin and Its Pt(II) Complexâ€‘ Synthesis, Cytotoxicity and Xanthine Oxidase Inhibitory Activity. <i>Inorganics</i> , 2022, 10, 175. | 1.2 | 1 |
| 16982 | Comparison of Density-Matrix Corrections to Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 6600-6607. | 2.3 | 9 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 16983 | Transition state search and geometry relaxation throughout chemical compound space with quantum machine learning. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 7 |
| 16984 | Experimental and Theoretical Study on the Homodimerization Mechanism of 3-Acetylcoumarin. <i>Molecules</i> , 2022, 27, 7228. | 1.7 | 0 |
| 16985 | Bifacial Dye Membranes: Ultrathin and Free-standing although not Being Covalently Bound. <i>Advanced Materials</i> , 2023, 35, . | 11.1 | 3 |
| 16986 | New gold(III) chlorophenyl terpyridine complex: Biomolecular interactions and anticancer activity against human oral squamous cell carcinoma. <i>Applied Organometallic Chemistry</i> , 2023, 37, . | 1.7 | 2 |
| 16987 | Constitutional isomerism of the linkages in donor-acceptor covalent organic frameworks and its impact on photocatalysis. <i>Nature Communications</i> , 2022, 13, . | 5.8 | 63 |
| 16988 | Reorganization Energies for Interfacial Proton-Coupled Electron Transfer to a Water Oxidation Catalyst. <i>Journal of the American Chemical Society</i> , 2022, 144, 20514-20524. | 6.6 | 7 |
| 16989 | An Ab Initio Investigation on Relevant Oligomerization Reactions of Toluene Diisocyanate (TDI). <i>Polymers</i> , 2022, 14, 4183. | 2.0 | 1 |
| 16990 | Efficient synthesis of new azo-sulfonamide derivatives and investigation of their molecular docking and cytotoxicity results. <i>Arabian Journal of Chemistry</i> , 2022, 15, 104383. | 2.3 | 7 |
| 16991 | Unique Reaction of Cyclicimides Containing Double Bond with Chlorosulfonyl isocyanate and theoretical computations: Solvent-free Reactions. <i>Journal of Molecular Structure</i> , 2022, , 134428. | 1.8 | 0 |
| 16992 | Synthesis of Sterically Encumbered Thiourea Oxides through Direct Thiourea Oxidation. <i>Chemistry - A European Journal</i> , 2023, 29, . | 1.7 | 3 |
| 16993 | Ab Initio Study of Hydrogen Bond Dynamics in Three-Component Crystals Comprising (DABCOH) _n Polycationic Chains. <i>ChemPhysChem</i> , 2023, 24, . | 1.0 | 0 |
| 16994 | C ₃ -Symmetric Propeller-like Phenanthridine Derivative with Multiple Write-In Modes for Programmable Anti-Counterfeiting. <i>Chemistry of Materials</i> , 2022, 34, 9492-9502. | 3.2 | 7 |
| 16995 | Impact of the Cellular Environment on Adenosine Triphosphate Conformations. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 9809-9814. | 2.1 | 2 |
| 16996 | Exploration of Dihydrothieno[2,3-c] Isoquinolines As Luminescent Materials and Corrosion Inhibitors. <i>ACS Omega</i> , 2022, 7, 38389-38399. | 1.6 | 2 |
| 16997 | Synchronous Doping Effects of Cathode Interlayers on Efficient Organic Solar Cells. <i>ACS Energy Letters</i> , 2022, 7, 4052-4060. | 8.8 | 16 |
| 16998 | Many recent density functionals are numerically ill-behaved. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 14 |
| 16999 | Synergism of 2-mercaptobenzimidazole and oleic imidazoline on corrosion inhibition of carbon steel in CO ₂ -saturated brine solutions. <i>Journal of Molecular Liquids</i> , 2022, 368, 120645. | 2.3 | 7 |
| 17000 | Ligand additivity relationships enable efficient exploration of transition metal chemical space. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 6 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 17001 | Microbial Denitrification: Active Site and Reaction Path Models Predict New Isotopic Fingerprints. ACS Earth and Space Chemistry, 2022, 6, 2582-2594. | 1.2 | 1 |
| 17002 | Effects of Nitrate Radical Levels and Pre-Existing Particles on Secondary Brown Carbon Formation from Nighttime Oxidation of Furan. ACS Earth and Space Chemistry, 2022, 6, 2709-2721. | 1.2 | 3 |
| 17003 | Mechanistic insights into CO ₂ conversion chemistry of copper bis-(terpyridine) molecular electrocatalyst using accessible operando spectrochemistry. Nature Communications, 2022, 13, . | 5.8 | 24 |
| 17004 | Reliable Isotropic Electron-Paramagnetic-Resonance Hyperfine Coupling Constants from the Frozen-Density Embedding Quasi-Diabatization Approach. Journal of Physical Chemistry A, 2022, 126, 8358-8368. | 1.1 | 1 |
| 17005 | Tools for Understanding and Predicting the Affinity of Per- and Polyfluoroalkyl Substances for Anion-Exchange Sorbents. Environmental Science & Technology, 2022, 56, 15470-15477. | 4.6 | 9 |
| 17006 | Acceleration of Nonradiative Charge Recombination Reactions at Larger Distances in Kinked Donor-“Bridge”-Acceptor Molecules. Journal of Physical Chemistry B, 2022, 126, 8851-8863. | 1.2 | 0 |
| 17007 | High-Energy and Insensitive Tetrazole-Substituted 2,5-Dinitroiminooctahydroimidazo[4,5- <i>d</i>]imidazole: Synthesis, Characterization, and Energetic Properties. Crystal Growth and Design, 2022, 22, 6952-6959. | 1.4 | 0 |
| 17008 | Predicting Regioselectivity of AO, CYP, FMO, and UGT Metabolism Using Quantum Mechanical Simulations and Machine Learning. Journal of Medicinal Chemistry, 2022, 65, 14066-14081. | 2.9 | 10 |
| 17009 | Polarizable MD and QM/MM investigation of acrylamide-based leads to target the main protease of SARS-CoV-2. Journal of Chemical Physics, 2022, 157, . | 1.2 | 3 |
| 17010 | Cheminformatics Study on Structural and Bactericidal Activity of Latest Generation Î ² -Lactams on Widespread Pathogens. International Journal of Molecular Sciences, 2022, 23, 12685. | 1.8 | 0 |
| 17011 | Synthesis, characterization, DFT calculations and bromoperoxidase activity of binuclear oxidovanadium complexes containing vitamin B6. Journal of Coordination Chemistry, 0, , 1-22. | 0.8 | 0 |
| 17012 | Homogeneous Electrocatalytic Reduction of CO ₂ by a CrN ₃ O Complex: Electronic Coupling with a Redox-Active Terpyridine Fragment Favors Selectivity for CO. Inorganic Chemistry, 2022, 61, 16963-16970. | 1.9 | 5 |
| 17013 | Aromaticity of the Triplet States of Corannulene and Coronene. Journal of Physical Organic Chemistry, 0, , . | 0.9 | 1 |
| 17014 | Medium effects on the fluorescence of Imide-substituted naphthalene diimides. Journal of Photochemistry and Photobiology A: Chemistry, 2023, 436, 114364. | 2.0 | 6 |
| 17015 | Binding of an Electron by a Finite Fixed Dipole. Journal of Physical Chemistry Letters, 2022, 13, 10331-10334. | 2.1 | 5 |
| 17016 | Efficient Activity Enhancement of a Lipase from <i>Sporisorium reilianum</i> for the Synthesis of a Moxifloxacin Chiral Intermediate via Rational Design. Engineering, 2022, , . | 3.2 | 1 |
| 17017 | Helicene Structure between DNA and Cyanuric Acid: The Role of Noncovalent Interactions. Journal of Physical Chemistry B, 2022, 126, 8508-8514. | 1.2 | 2 |
| 17018 | When Gold Is Not Enough: Platinum Standard of Quantum Chemistry with <i>N</i> ⁷ Cost. Journal of Chemical Theory and Computation, 2022, 18, 6537-6556. | 2.3 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 17019 | A General Strategy for Radical Ring-Opening Polymerization of Macrocyclic Allylic Sulfides. <i>Macromolecules</i> , 2022, 55, 9411-9419. | 2.2 | 10 |
| 17020 | Investigations of an Unexpected [2+2] Photocycloaddition in the Synthesis of (âˆ™)-Scabrolide A from Quantum Mechanics Calculations. <i>Journal of Organic Chemistry</i> , 2022, 87, 14115-14124. | 1.7 | 3 |
| 17021 | Molecular-orbital-based machine learning for open-shell and multi-reference systems with kernel addition Gaussian process regression. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 3 |
| 17022 | High Resolution Photoelectron Spectroscopy of the Acetyl Anion. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7962-7970. | 1.1 | 5 |
| 17023 | Effects of Heterogeneous Protein Environment on Excitation Energy Transfer Dynamics in the Fennaâ€“Matthewsâ€“Olson Complex. <i>Journal of Physical Chemistry B</i> , 2022, 126, 9271-9287. | 1.2 | 3 |
| 17024 | Degradation of Quinoneâ€“based Flow Battery Electrolytes: Effect of Functional Groups on the Reaction Mechanism**. <i>Batteries and Supercaps</i> , 2023, 6, . | 2.4 | 0 |
| 17025 | Synthesis, characterization, and biological activities of zinc(II), copper(II) and nickel(II) complexes of an aminoquinoline derivative. <i>Frontiers in Chemistry</i> , 0, 10, . | 1.8 | 4 |
| 17026 | Pyrrolidine-2,5-dione-derived ionic liquids promoted efficient transformation of flue gas CO2 into \pm -alkylidene cyclic carbonates at room temperature. <i>Journal of CO2 Utilization</i> , 2022, 65, 102227. | 3.3 | 2 |
| 17027 | The Accuracy of Semi-Empirical Quantum Chemistry Methods on Soot Formation Simulation. <i>International Journal of Molecular Sciences</i> , 2022, 23, 13371. | 1.8 | 1 |
| 17028 | Palladium/PCâ€“Phosâ€“Catalyzed Asymmetric Heck/Tsujiâ€“Trost Reactions of Aminoâ€“Tethered 1,3â€“Cyclohexadiene with Aryl and Alkenyl Halides. <i>Angewandte Chemie</i> , 0, , . | 1.6 | 0 |
| 17029 | Azaboracyclooctatetraenes reveal that the different aspects of triplet state Bairdâ€“aromaticity are nothing but different. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, . | 0.9 | 6 |
| 17030 | Palladium/PCâ€“Phosâ€“Catalyzed Asymmetric Heck/Tsujiâ€“Trost Reactions of Aminoâ€“Tethered 1,3â€“Cyclohexadiene with Aryl and Alkenyl Halides. <i>Angewandte Chemie - International Edition</i> , 2023, 62, . | 7.2 | 7 |
| 17031 | Synthesis, spectral characterization, DFT and in silico ADME studies of the novel pyrido[1,2-a]benzimidazoles and pyrazolo[3,4-b]pyridines. <i>Journal of Molecular Structure</i> , 2023, 1274, 134454. | 1.8 | 8 |
| 17032 | Kinetics of the RÂˆ+ÂˆO2Âˆ+ÂˆRÂˆ+â€“HOÂˆ+ÂˆOH reactions of substituted methyl radicals: Effects of Cl, F, and CF3 substitution and notes on the ROÂˆ+ÂˆO producing channel. <i>Chemical Physics Letters</i> , 2022, 808, 140121. | 1.2 | 1 |
| 17033 | Application for the porous structure of cellulose separators: Ionic conduction path in lithium-ion battery. <i>Journal of Electroanalytical Chemistry</i> , 2022, 926, 116937. | 1.9 | 1 |
| 17034 | Effect of hydroxyl functional groups on SO2 adsorption by activated carbon. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108727. | 3.3 | 4 |
| 17035 | La(III) loaded Fe(III) crossâ€“linked chitosan composites for efficient removal of phosphate from wastewater: Performance and mechanisms. <i>Journal of Cleaner Production</i> , 2022, 379, 134833. | 4.6 | 14 |
| 17036 | Difference in the hydration state of water at the hydrophobic interface of structural isomers of propanol investigated by U.V visible absorption and Raman spectroscopic study. <i>Journal of Molecular Liquids</i> , 2022, 368, 120530. | 2.3 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17037 | Chemo-enzymatic synthesis of sugar acid by pyranose 2-oxidase. <i>Molecular Catalysis</i> , 2022, 533, 112753. | 1.0 | 1 |
| 17038 | Substituent effects in carbon-nanotube-supported diiron monophosphine complexes for hydrogen evolution reaction. <i>Electrochimica Acta</i> , 2022, 434, 141325. | 2.6 | 3 |
| 17039 | DFT Insights into the mechanism of Ru(II) Catalyzed C7-selective amidation of N-pivaloylindole. <i>Journal of Organometallic Chemistry</i> , 2022, 982, 122534. | 0.8 | 1 |
| 17040 | Theoretical study of multi-coordinated Xe(AuF) ($n=4$): Intriguing bond-bending isomerism. <i>Chemical Physics</i> , 2023, 565, 111743. | 0.9 | 1 |
| 17041 | Evidence of molecular clicking on self-assembled monolayers on Au (111) and their properties. <i>Computational Materials Science</i> , 2023, 216, 111809. | 1.4 | 0 |
| 17042 | Molecular electrides: An overview of their structure, bonding, and reactivity. , 2023, , 275-295. | | 0 |
| 17043 | Potential of HF and CO ₂ loss through dissociative electron attachment to increase radiosensitizers reactivity; case study on pentafluorobenzoic acid. <i>Radiation Physics and Chemistry</i> , 2023, 202, 110544. | 1.4 | 3 |
| 17044 | Demystifying viscous isoalkanes as the organic solvent in interfacial polymerization for manufacturing desalination membranes. <i>Desalination</i> , 2023, 545, 116166. | 4.0 | 3 |
| 17045 | Molecular structure, spectral and theoretical study of new type bile acid-sterol conjugates linked via 1,2,3-triazole ring. <i>Journal of Molecular Structure</i> , 2023, 1273, 134313. | 1.8 | 2 |
| 17046 | Binding of ion pairs and neutral guests by aryl-extended meso- <i>p</i> -hydroxyphenyl calix[4]pyrrole: The interplay between three binding sites. <i>Journal of Molecular Structure</i> , 2023, 1273, 134268. | 1.8 | 3 |
| 17047 | A theoretical investigation of the possible mechanisms for detection the copper ions by a retinal-base sensor. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 436, 114363. | 2.0 | 1 |
| 17048 | Tropine-based dicationic molten salt: An active catalyst in the acceleration of one-pot synthesis of spiro-2-amino-4H-pyran-oxindoles and bis-2-amino-4H-pyrans. <i>Journal of Molecular Structure</i> , 2023, 1274, 134410. | 1.8 | 1 |
| 17049 | Design and development of imidazo[4,5-f] [1,10] phenanthroline-Zn(II) based fluorescent probes for specific recognition of ATP with tunable optical responses and probing the enzymatic hydrolysis of ATP by alkaline phosphatase. <i>New Journal of Chemistry</i> , 2022, 46, 23139-23154. | 1.4 | 3 |
| 17050 | Electron diffraction of 1,4-dichlorobenzene embedded in superfluid helium droplets. <i>Physical Chemistry Chemical Physics</i> , 0, , . | 1.3 | 0 |
| 17051 | A combined photobiological-photochemical route to C ₁₀ cycloalkane jet fuels from carbon dioxide via isoprene. <i>Green Chemistry</i> , 2022, 24, 9602-9619. | 4.6 | 14 |
| 17052 | Control of spin coupling through a redox-active bridge in a dinickel(II) porphyrin dimer: step-wise oxidations enable isolations of a chlorin-porphyrin heterodimer and a dication diradical with a singlet ground state. <i>Dalton Transactions</i> , 2023, 52, 877-891. | 1.6 | 2 |
| 17053 | Theoretical exploration of molecular packing and the charge transfer mechanism of organic solar cells based on PM6:Y6. <i>Journal of Materials Chemistry A</i> , 2022, 10, 25611-25619. | 5.2 | 6 |
| 17054 | Antioxidant mechanisms and products of four 4 ² ,5,7-trihydroxyflavonoids with different structural types. <i>RSC Medicinal Chemistry</i> , 2023, 14, 173-182. | 1.7 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17055 | Uniaxial strain tuning of organic molecule single photon sources. <i>Nanoscale</i> , 2022, 15, 177-184. | 2.8 | 1 |
| 17056 | Near-infrared electroluminescence beyond 940 nm in Pt(N ^C N)X complexes: influencing aggregation with the ancillary ligand X. <i>Chemical Science</i> , 2022, 13, 13600-13610. | 3.7 | 12 |
| 17057 | Mechanistic investigation of char growth from lignin monomers during biomass utilisation. <i>Fuel Processing Technology</i> , 2023, 239, 107556. | 3.7 | 4 |
| 17058 | Diffusion Monte Carlo investigation of electronic structure properties for 13-atom alkali metal clusters. <i>Chemical Physics</i> , 2023, 565, 111767. | 0.9 | 0 |
| 17059 | Novel assessment of highly efficient polyamines for post-combustion CO ₂ capture: Absorption heat, reaction rate, CO ₂ cyclic capacity, and phase change behavior. <i>Separation and Purification Technology</i> , 2023, 306, 122615. | 3.9 | 22 |
| 17060 | A novel pH-Dependent sensor for recognition of strontium ions in water: A hierarchically structured mesoporous architectonics. <i>Talanta</i> , 2023, 253, 124064. | 2.9 | 1 |
| 17061 | Novel insights on the graphene oxide nanosheets induced demulsification and emulsification of crude oil-in-water emulsion: A molecular simulation study. <i>Fuel</i> , 2023, 333, 126529. | 3.4 | 3 |
| 17062 | Experimental and computational study on dimers of 5-halo-1H-indole-2-carboxylic acids and their microbiological activity. <i>Journal of Molecular Structure</i> , 2023, 1274, 134492. | 1.8 | 4 |
| 17063 | Heterodimetallic iridium-rhenium system: Synthesis, computational and photocatalytic aspects. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 436, 114407. | 2.0 | 1 |
| 17064 | Synthesis, characterization, theoretical studies and antioxidant and cytotoxic evaluation of a series of Tetrahydrocurcumin (THC)-benzylated derivatives. <i>Journal of Molecular Structure</i> , 2023, 1273, 134355. | 1.8 | 2 |
| 17065 | Assessment of advanced xDH@B3LYP methods in describing various potential energy curves driven by π - π , CH \cdots π , and SH \cdots π non-bonded interactions. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 720-726. | 0.6 | 2 |
| 17066 | Reactions of dimedone and alkyl orthoformates with and without activators. <i>Russian Chemical Bulletin</i> , 2022, 71, 2241-2254. | 0.4 | 1 |
| 17067 | π -Expanded pyrazinoporphyrins for photocatalysis: How many rings are required?. <i>Dyes and Pigments</i> , 2023, 210, 110935. | 2.0 | 3 |
| 17068 | Copper-Catalyzed Homocoupling of Boronic Acids: A Focus on B-to-Cu and Cu-to-Cu Transmetalations. <i>Molecules</i> , 2022, 27, 7517. | 1.7 | 2 |
| 17069 | Unprecedented cleavage of -N-N- bond of ligand and phenyl ring nitration during nitric oxide (NO) reactivity studies: new ruthenium nitrosyl complex and photoinduced liberation of NO. <i>Journal of Coordination Chemistry</i> , 0, , 1-11. | 0.8 | 1 |
| 17070 | An experimental and theoretical study on the effects of amine chain length on CO_2 absorption performance. <i>AIChE Journal</i> , 2023, 69, . | 1.8 | 8 |
| 17071 | Application of Multiconfiguration Pair-Density Functional Theory to the Diels-Alder Reaction. <i>Journal of Physical Chemistry A</i> , 2022, 126, 8834-8843. | 1.1 | 1 |
| 17072 | Predicting Small Molecule Activation including Catalytic Hydrogenation of Dinitrogen Promoted by a Dual Lewis Acid. <i>Chemistry - an Asian Journal</i> , 2023, 18, . | 1.7 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17073 | Extracting Inelastic Scattering Cross Sections for Finite and Aperiodic Materials from Electronic Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 0, , . | 2.3 | 0 |
| 17074 | Synthesis, characterization and computational investigation of the phosphatase activity of a dinuclear Zinc(II) complex containing a new heptadentate asymmetric ligand. <i>Journal of Inorganic Biochemistry</i> , 2022, , 112064. | 1.5 | 1 |
| 17075 | Effects of Fluorinated Aromatic Spacer in Ag ⁺ /Bi Double Perovskite for X-ray Detector. <i>Journal of Physical Chemistry C</i> , 2022, 126, 19417-19423. | 1.5 | 6 |
| 17076 | Experimental Detection and Simulation of Terahertz Spectra of Aqueous L-Arginine. <i>Biosensors</i> , 2022, 12, 1029. | 2.3 | 1 |
| 17077 | Synthesis, spectral characterization and fluorescence study of functional [5]Helicene derivatives: Experimental and theoretical investigation. <i>Journal of Molecular Structure</i> , 2022, , 134574. | 1.8 | 0 |
| 17078 | Variable Dimensionality of Europium(III) and Terbium(III) Coordination Compounds with a Flexible Hexacarboxylate Ligand. <i>Molecules</i> , 2022, 27, 7849. | 1.7 | 3 |
| 17079 | Comprehensive evaluation of end-point free energy techniques in carboxylated-pillar[6]arene host-guest binding: II. regression and dielectric constant. <i>Journal of Computer-Aided Molecular Design</i> , 2022, 36, 879-894. | 1.3 | 7 |
| 17080 | Strategies to Enhance the Rate of Proton-Coupled Electron Transfer Reactions in Dye-Water Oxidation Catalyst Complexes. <i>ChemPhotoChem</i> , 0, , . | 1.5 | 0 |
| 17081 | Electronic Substitution Effect on the Ground and Excited State Properties of Indole Chromophore: A Computational Study**. <i>ChemPhysChem</i> , 2023, 24, . | 1.0 | 3 |
| 17082 | Tetranuclear Copper Complexes with Bulky Aminoalcohol Ligands as Catalysts for Oxidative Phenoxazinone Synthase-like Coupling of Aminophenol: A Combined Experimental and Theoretical Study. <i>Catalysts</i> , 2022, 12, 1408. | 1.6 | 3 |
| 17083 | Atroposelective Synthesis of Tetrahydropyrrolo[3,2- <i>b</i>]azepine Derivatives Through Gold(I)-Catalyzed Hydroarylation. <i>Advanced Synthesis and Catalysis</i> , 0, , . | 2.1 | 1 |
| 17084 | Electrocatalytic CO ₂ reduction with a binuclear bis-terpyridine pyrazole-bridged cobalt complex. <i>Chemistry - A European Journal</i> , 0, , . | 1.7 | 2 |
| 17085 | High-level quantum chemistry exploration of reduction by group-13 hydrides: insights into the rational design of bio-mimic CO ₂ reduction. <i>Electronic Structure</i> , 2022, 4, 044001. | 1.0 | 0 |
| 17086 | Advanced polyimide separator via co-precursor method for lithium-ion batteries with low thermal runaway risks. <i>Journal of Energy Storage</i> , 2022, 56, 106100. | 3.9 | 4 |
| 17087 | Single crystal structure feature and quantum mechanical studies of a new binuclear Bi (III) complex and its activity against <i>Helicobacter pylori</i> . <i>Inorganic Chemistry Communication</i> , 2022, 146, 110207. | 1.8 | 1 |
| 17088 | Generalization of ETS-NOCV and ALMO-COVP Energy Decomposition Analysis to Connect Any Two Electronic States and Comparative Assessment. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 7428-7441. | 2.3 | 5 |
| 17089 | Disproportionation and Ligand Lability in Low Oxidation State Boryl-Tin Chemistry**. <i>Chemistry - A European Journal</i> , 2023, 29, . | 1.7 | 6 |
| 17090 | Vertex effects in describing the ionization energies of the first-row transition-metal monoxide molecules. <i>Journal of Chemical Physics</i> , 2022, 157, . | 1.2 | 8 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 17091 | Photodissociation Dynamics of CF ₂ ClCHFI Using Slice Imaging Combined with a Hexapole-Oriented Molecular Beam. <i>Journal of Physical Chemistry A</i> , 2022, 126, 8844-8850. | 1.1 | 1 |
| 17092 | Mechanical nanolattices printed using nanocluster-based photoresists. <i>Science</i> , 2022, 378, 768-773. | 6.0 | 20 |
| 17093 | Quantum DFT methods to explore the interaction of 1-Adamantylamine with pristine, and P, As, Al, and Ga doped BN nanotubes. <i>Scientific Reports</i> , 2022, 12, . | 1.6 | 5 |
| 17094 | Intrinsic influence of selenium substitution in thiophene and benzo-2,1,3-thiadiazole on the electronic structure, excited states and photovoltaic performances evaluated using theoretical calculations. <i>New Journal of Chemistry</i> , 2023, 47, 1797-1807. | 1.4 | 5 |
| 17095 | Why does the synthesis of N-phenylbenzamide from benzenesulfinate and phenylisocyanate via the palladium-mediated Extrusion-Insertion pathway not work? A mechanistic exploration. <i>Australian Journal of Chemistry</i> , 2022, , . | 0.5 | 2 |
| 17096 | Design, synthesis, theoretical study, antioxidant, and anticholinesterase activities of new pyrazolo-fused phenanthrolines. <i>RSC Advances</i> , 2022, 12, 33032-33048. | 1.7 | 2 |
| 17097 | Benchmarking the quadrupolar coupling tensor for chlorine to probe weak-bonding interactions. <i>Physical Chemistry Chemical Physics</i> , 0, , . | 1.3 | 0 |
| 17098 | A critical comparison of CH-π versus π-π interactions in the benzene dimer: obtaining benchmarks at the CCSD(T) level and assessing the accuracy of lower scaling methods. <i>Physical Chemistry Chemical Physics</i> , 0, , . | 1.3 | 0 |
| 17099 | A TD-DFT study of a class of D-π-A fluorescent probes for detection of typical oxidants. <i>Organic and Biomolecular Chemistry</i> , 2023, 21, 315-322. | 1.5 | 2 |
| 17100 | Enhanced circularly polarized luminescence of chiral Eu(III) coordination polymers with structural strain. <i>Dalton Transactions</i> , 0, , . | 1.6 | 3 |
| 17101 | Predicting adsorption behavior of Triacanthine anticancer drug with pure B12N12 nano-cage: A theoretical study. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100812. | 1.3 | 4 |
| 17102 | Theoretical investigation on intermolecular interactions, co-crystal structure, thermal decomposition mechanism, and shock properties of 3-nitro-1,2,4-triazol-5-one (NTO) and ammonium perchlorate. <i>CrystEngComm</i> , 2023, 25, 671-682. | 1.3 | 4 |
| 17103 | Theoretical exploration to the significance of n(S)/n(O) → f* (C-COOMe) stereoelectronic interactions. <i>New Journal of Chemistry</i> , 2022, 47, 384-391. | 1.4 | 0 |
| 17104 | How to active ethanolamine for selective hydrogenation by imidazolium-based cation and conjugated π bond. <i>Molecular Catalysis</i> , 2023, 535, 112809. | 1.0 | 0 |
| 17105 | Quinoxaline-fused octaphyrin(2.0.0.0.2.0.0.0). A rudimentary chemosensor. <i>Chemical Communications</i> , 2023, 59, 708-711. | 2.2 | 2 |
| 17106 | Quantum chemistry insight into the interactions of 1,3-diisopropoxycalix[4]arene-crown-6 with alkali metal cations: Structure, selectivity, and solvation. <i>Journal of Molecular Liquids</i> , 2023, 370, 121054. | 2.3 | 4 |
| 17107 | π-π stacking in the polymorphism of 2-(naphthalenylamino)-nicotinic acids and a comparison with their analogues. <i>CrystEngComm</i> , 2023, 25, 432-443. | 1.3 | 1 |
| 17108 | Engineering aluminosilicate's photochromism by quantum chemistry. <i>Journal of Materials Chemistry C</i> , 2023, 11, 730-741. | 2.7 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17109 | Complexation of sodium sulfamerazine with an ionic resorcin[4]arene: Thermodynamic and computational study. <i>Journal of Molecular Liquids</i> , 2023, 370, 120954. | 2.3 | 1 |
| 17110 | Incorporating self-healing capability in temperature-sensitive hydrogels by non-covalent chitosan crosslinkers. <i>European Polymer Journal</i> , 2023, 182, 111728. | 2.6 | 7 |
| 17111 | New ruthenium(II) complexes with quinone diimine and substituted bipyridine as inert ligands: synthesis, characterization, mechanism of action, DNA/HSA binding affinity and cytotoxic activity. <i>Dalton Transactions</i> , 2023, 52, 1323-1344. | 1.6 | 6 |
| 17112 | Cu(I)-catalysed asymmetric intramolecular tandem oxaziridination/rearrangement reaction: theoretical insight into the mechanism, enantioselectivity, ligand effect, and comparison with the corresponding Lewis-acid-promoted reaction. <i>Organic Chemistry Frontiers</i> , 0, , . | 2.3 | 0 |
| 17113 | A theoretical framework for the design of molecular crystal engines. <i>Chemical Science</i> , 2023, 14, 937-949. | 3.7 | 7 |
| 17114 | Electronic structures of zwitterionic and protonated forms of glycine betaine in water: Insights into solvent effects from ab initio simulations. <i>Journal of Molecular Liquids</i> , 2023, 369, 120871. | 2.3 | 5 |
| 17115 | Magneto-structural correlations of dinickel(II) complexes with phenoxido/azido coligands: A theoretical investigation. <i>Chemical Physics Letters</i> , 2023, 811, 140241. | 1.2 | 2 |
| 17116 | Thermogalvanic hydrogel electrolyte for harvesting biothermal energy enabled by a novel redox couple of SO ₄ ²⁻ /SO ₃ ²⁻ ions. <i>Nano Energy</i> , 2023, 106, 108077. | 8.2 | 24 |
| 17117 | Theoretical study on the vibrational structures in the conductance spectra of a weakly coupled polycyclic aromatic hydrocarbon molecule. <i>Chemical Physics Letters</i> , 2023, 812, 140272. | 1.2 | 0 |
| 17118 | Ag ⁺ ion in choline chloride and glycerol mixture: Evaluation of electrochemical properties and molecular modelling approaches. <i>Journal of Molecular Liquids</i> , 2023, 371, 121053. | 2.3 | 4 |
| 17119 | A quantum-chemical study of boro-fullerenes B ₆₀ H ₆₀ , B ₆₀ F ₃₀ H ₃₀ , and B ₆₀ F ₆₀ . <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 113987. | 1.1 | 0 |
| 17120 | The simultaneous elimination of arsenic and mercury ions via hollow fiber supported liquid membrane and their reaction mechanisms: Experimental and modeling based on DFT and generating function. <i>Arabian Journal of Chemistry</i> , 2023, 16, 104501. | 2.3 | 5 |
| 17121 | A QSPR study for predicting \hat{T}_g (LCST) and \hat{T}_g (UCST) in binary polymer solutions. <i>Chemical Engineering Science</i> , 2023, 267, 118326. | 1.9 | 6 |
| 17122 | Effective removal of Hg ²⁺ and Cd ²⁺ in aqueous systems by Fe-Mn oxide modified biochar: A combined experimental and DFT calculation. <i>Desalination</i> , 2023, 549, 116306. | 4.0 | 14 |
| 17123 | Crystal structure, IR and NMR spectra of (E)-2-methoxy-4-(2-morpholinovinyl)phenol molecule and its DFT calculations. <i>Journal of Molecular Structure</i> , 2023, 1275, 134669. | 1.8 | 2 |
| 17124 | A combined experimental and computational thermodynamic study of fluoronitrophenol isomers. <i>Journal of Chemical Thermodynamics</i> , 2023, 178, 106954. | 1.0 | 0 |
| 17125 | Electron scattering and ionization of astrophysical molecules. <i>Radiation Physics and Chemistry</i> , 2023, 204, 110686. | 1.4 | 0 |
| 17126 | Photocatalytic degradation of phenol and its derivatives over ZnFe layered double hydroxide. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 438, 114509. | 2.0 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 17127 | Structural modification and band gap engineering of carbon nano-onions via sulphur doping: Theoretical DFT study. <i>Applied Surface Science</i> , 2023, 613, 156046. | 3.1 | 2 |
| 17128 | Adsorption mechanism of ammonia nitrogen and phenol on lignite surface: Molecular dynamics simulations and quantum chemical calculations. <i>Fuel</i> , 2023, 337, 127157. | 3.4 | 4 |
| 17129 | Experimental evidence and computational results in the investigation of thermodynamic properties and molecular structure of hydrogen-bonded cyclohexylamine and ethyl methyl ketone system. <i>Journal of Chemical Thermodynamics</i> , 2023, 179, 106984. | 1.0 | 4 |
| 17130 | Fragmentation modeling of gas-phase ionic liquid clusters in high-voltage electric field. <i>Fuel</i> , 2023, 335, 126919. | 3.4 | 2 |
| 17131 | A DFT study of the <i>endo</i> -selectivity mechanism of the Diels-Alder reaction in lindenane dimeric sesquiterpene synthesis promoted by pyridines. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 3772-3779. | 1.3 | 1 |
| 17132 | A turn-on bis-BODIPY chemosensor for copper recognition based on the <i>in situ</i> generation of a benzimidazole-triazole receptor and its applications in bioimaging. <i>New Journal of Chemistry</i> , 2022, 46, 22525-22532. | 1.4 | 5 |
| 17133 | Self-diffusion and molecular association in the binary systems dimethyl sulfoxide-chloroform and acetone-chloroform. <i>Results in Chemistry</i> , 2022, 4, 100673. | 0.9 | 1 |
| 17134 | Sustainable Synthesis of Benzylidenemalononitrile Compounds Under Microwave-Irradiation. <i>Current Organic Chemistry</i> , 2022, 26, 1552-1564. | 0.9 | 0 |
| 17135 | Influence of the metal-support and metal-metal interactions on Pd nucleation and NO adsorption in a Pd ₄ /γ-Al ₂ O ₃ (110D) model. <i>Journal of Molecular Modeling</i> , 2022, 28, . | 0.8 | 1 |
| 17136 | Investigation for Carbonation Mechanism of Tobermorite 9 Å...: A Combination of DFT and Ab Initio Molecular Dynamics Study. <i>Advanced Theory and Simulations</i> , 0, , 2200729. | 1.3 | 0 |
| 17137 | Coordinative Combination of Nitroamine and Gem-Dinitromethyl with Fused Ring for Enhanced Oxygen Balances and Detonation Properties. <i>International Journal of Molecular Sciences</i> , 2022, 23, 14337. | 1.8 | 0 |
| 17138 | Examining the Long-Range Effect in Very Long Graphene Nanoribbons: A First-Principles Study. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 11223-11229. | 2.1 | 0 |
| 17139 | Molecular Design of the Polyamide Layer Structure of Nanofiltration Membranes by Sacrificing Hydrolyzable Groups toward Enhanced Separation Performance. <i>Environmental Science & Technology</i> , 2022, 56, 17955-17964. | 4.6 | 11 |
| 17140 | Fabrication of a Molecularly Imprinted Nano-Interface-Based Electrochemical Biosensor for the Detection of CagA Virulence Factors of <i>H. pylori</i> . <i>Biosensors</i> , 2022, 12, 1066. | 2.3 | 5 |
| 17141 | A Simplified Treatment for Efficiently Modeling the Spectral Signal of Vibronic Transitions: Application to Aqueous Indole. <i>Molecules</i> , 2022, 27, 8135. | 1.7 | 3 |
| 17142 | Protocols for Understanding the Redox Behavior of Copper-Containing Systems. <i>ACS Omega</i> , 2022, 7, 45057-45066. | 1.6 | 2 |
| 17143 | Biomimetic Approach toward Visible Light-Driven Hydrogen Generation Based on a Porphyrin-Based Coordination Polymer Gel. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 25173-25183. | 4.0 | 6 |
| 17144 | Effects of Through-Bond and Through-Space Conjugations on the Photoluminescence of Small Aromatic and Aliphatic Aldimines. <i>Molecules</i> , 2022, 27, 8046. | 1.7 | 5 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17145 | The Origin of Stereoselectivity in the Hydrogenation of Oximes Catalyzed by Iridium Complexes: A DFT Mechanistic Study. <i>Molecules</i> , 2022, 27, 8349. | 1.7 | 2 |
| 17146 | [3 + 2]-Cycloadditions with Porphyrin π^2, π^2 -Bonds: Theoretical Basis of the Counterintuitive <i>meso</i> -Aryl Group Influence on the Rates of Reaction. <i>Journal of Organic Chemistry</i> , 2022, 87, 16473-16482. | 1.7 | 1 |
| 17147 | $\hat{\pi}$ -Methylstilbene Isomers: Relationship of Structure to Photophysics and Photochemistry. <i>Journal of Physical Chemistry A</i> , 2022, 126, 8976-8987. | 1.1 | 3 |
| 17148 | From Molecules to Heat-Integrated Processes: Computer-Aided Design of Solvents and Processes Using Quantum Chemistry. <i>Chemie-Ingenieur-Technik</i> , 0, , . | 0.4 | 2 |
| 17149 | Duplex DNA Retains the Conformational Features of Single Strands: Perspectives from MD Simulations and Quantum Chemical Computations. <i>International Journal of Molecular Sciences</i> , 2022, 23, 14452. | 1.8 | 2 |
| 17150 | Two Theorems and Important Insight on How the Preferred Mechanism of Free Radical Scavenging Cannot Be Settled. Comment on Pandithavidana, D.R.; Jayawardana, S.B. Comparative Study of Antioxidant Potential of Selected Dietary Vitamins; Computational Insights. <i>Molecules</i> 2019, 24, 1646. <i>Molecules</i> , 2022, 27, 8092. | 1.7 | 4 |
| 17151 | Development of QSRR model for hydroxamic acids using PCA-GA-BP algorithm incorporated with molecular interaction-based features. <i>Frontiers in Chemistry</i> , 0, 10, . | 1.8 | 2 |
| 17152 | Symmetry analysis of irregular objects. <i>Journal of Mathematical Chemistry</i> , 2023, 61, 504-519. | 0.7 | 1 |
| 17153 | Collaborative Assessment of Molecular Geometries and Energies from the Open Force Field. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 6094-6104. | 2.5 | 7 |
| 17154 | Time-Dependent Density Functional Study of Nitrogen-Substituted Polycyclic Aromatic Hydrocarbons and Diffuse Interstellar Bands. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 2867-2876. | 1.2 | 1 |
| 17155 | Temperature, pressure, and adsorption-dependent redox potentials: α - γ . Processes of CH ₄ oxidation to value-added compounds. <i>Energy Science and Engineering</i> , 0, , . | 1.9 | 0 |
| 17156 | Effect of bridged spacers and auxiliary acceptors on <i>Dye Sensitized Solar Cell</i> sensitizers: A density functional theory-based investigation. <i>International Journal of Quantum Chemistry</i> , 2023, 123, . | 1.0 | 0 |
| 17157 | Synthesis and Physical Properties of Tunable Aryl Alkyl Ionic Liquids (TAAILs) Comprising Imidazolium Cations Blocked with Methyl-, Propyl- and Phenyl-Groups at the C2 Position. <i>Chemistry - A European Journal</i> , 2023, 29, . | 1.7 | 2 |
| 17158 | Consistent Evaluation of Magnetic Exchange Couplings in Multicenter Compounds in KS-DFT: The Recomposition Method. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 157-173. | 2.3 | 4 |
| 17159 | Hybrid Molecular Magnets with Lanthanide- and Countercation-Mediated Interfacial Electron Transfer between Phthalocyanine and Polyoxovanadate. <i>Inorganic Chemistry</i> , 2023, 62, 3761-3775. | 1.9 | 9 |
| 17160 | Catalytic Dehydrogenation of Liquid Organic Hydrogen Carrier Model Compounds by CpM ⁺ (M = Fe, Co, Ni) in the Gas Phase. <i>Organometallics</i> , 2022, 41, 3823-3833. | 1.1 | 2 |
| 17161 | Molecular Dynamics and Structural Studies of Zinc Chloroquine Complexes. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 161-172. | 2.5 | 4 |
| 17162 | Active Learning Exploration of Transition-Metal Complexes to Discover Method-Insensitive and Synthetically Accessible Chromophores. <i>Jacs Au</i> , 2023, 3, 391-401. | 3.6 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 17163 | Covalently Confined Sulfur Composite with Carbonized Bacterial Cellulose as an Efficient Cathode Matrix for High-Performance Potassium Sulfur Batteries. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 16634-16646. | 3.2 | 5 |
| 17164 | Selective Low-Level Detection of a Perilous Nitroaromatic Compound Using Tailor-Made Cd(II)-Based Coordination Polymers: Study of Photophysical Properties and Effect of Functional Groups. <i>Inorganic Chemistry</i> , 2023, 62, 98-113. | 1.9 | 11 |
| 17165 | An efficient approach to 3,4-fused β -lactone- β -lactams bicyclic moieties as anti-Alzheimer agents. <i>Structural Chemistry</i> , 2023, 34, 1577-1589. | 1.0 | 1 |
| 17166 | One-dimensional nanospace confinement effects on the chemical properties of organic molecules in carbon nanotubes: Quantum chemical calculation analyses. , 2022, 1, 175-187. | | 0 |
| 17167 | Mechanism and Origins of Diastereo- and Regioselectivities of Palladium-Catalyzed Remote Diborylative Cyclization of Dienes via Chain-Walking Strategy. <i>Chemistry - an Asian Journal</i> , 2023, 18, . | 1.7 | 2 |
| 17168 | Efficient Kohn-Sham density-functional theory implementation of isotropic spectroscopic observables associated with quadratic response functions. <i>Electronic Structure</i> , 2022, 4, 044004. | 1.0 | 0 |
| 17169 | Electronic, vibrational, and rotational analysis of 1,2-benzanthracene by high-resolution spectroscopy referenced to an optical frequency comb. <i>Journal of Chemical Physics</i> , 2022, 157, 234303. | 1.2 | 0 |
| 17170 | Solvent-Type Passivation Strategy Controls Solid-State Self-Quenching-Resistant Behavior in Sulfur Dots. <i>Inorganic Chemistry</i> , 2022, 61, 21157-21168. | 1.9 | 3 |
| 17171 | DFT Prediction of Radiolytic Stability of Conformationally Flexible Ligands. <i>Energies</i> , 2023, 16, 257. | 1.6 | 5 |
| 17172 | Benzo[1,4]diazocinone/Pyrrole Ensembles via the Catalyst-Free Insertion of Pyrrolylacetylenic Ketones into Benzimidazoles. <i>ChemistrySelect</i> , 2022, 7, . | 0.7 | 3 |
| 17173 | Probing into complexation and separation of chiral Curanium complex to chiral sulfur enantiomers R/S-ethiproles. <i>Applied Organometallic Chemistry</i> , 0, , . | 1.7 | 2 |
| 17174 | Molecular dynamics-based insight of VEGFR-2 kinase domain: a combined study of pharmacophore modeling and molecular docking and dynamics. <i>Journal of Molecular Modeling</i> , 2023, 29, . | 0.8 | 3 |
| 17175 | Mechanism study of the conductivity characteristics of cellulose electrical insulation influenced by moisture. <i>Journal of Applied Physics</i> , 2022, 132, 215104. | 1.1 | 0 |
| 17176 | HOMO-LUMO energy gaps of complexes of transition metals with single and multi-ring aromatics. <i>Combustion and Flame</i> , 2023, 257, 112513. | 2.8 | 3 |
| 17177 | Synthesis of Carrier-Free Paclitaxel-Curcumin Nanoparticles: The Role of Curcuminoids. <i>Bioengineering</i> , 2022, 9, 815. | 1.6 | 1 |
| 17178 | Non-innocent Role of the Halide Ligand in the Copper-Catalyzed Olefin Aziridination Reaction. <i>ACS Catalysis</i> , 2023, 13, 706-713. | 5.5 | 4 |
| 17179 | Glycolaldehyde formation mediated by interstellar amorphous ice: a computational study. <i>Monthly Notices of the Royal Astronomical Society</i> , 2022, 519, 2518-2527. | 1.6 | 2 |
| 17180 | Diheme cytochromes: Effect of mixed-axial ligation on the electronic structure and electrochemical properties with cobalt porphyrin dimer. <i>Journal of Inorganic Biochemistry</i> , 2023, 240, 112109. | 1.5 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17181 | Evidence of Graphene-like ZnO Nanostructures via Zinc Dimethoxide Hydrolysis-Condensation Under Ambient Conditions on a Au(111) Surface Using SERS: Simulation and Experiment. <i>Journal of Physical Chemistry C</i> , 2023, 127, 429-436. | 1.5 | 1 |
| 17182 | Anticancer Activity of Thiophene Carboxamide Derivatives as CA-4 Biomimetics: Synthesis, Biological Potency, 3D Spheroid Model, and Molecular Dynamics Simulation. <i>Biomimetics</i> , 2022, 7, 247. | 1.5 | 11 |
| 17183 | Sensitivity and Weak Interaction of Energetic Ionic Salts: An Example Case of $C_4N_{18}H_2$. <i>Crystal Growth and Design</i> , 2023, 23, 104-111. | 1.4 | 4 |
| 17184 | Solvent effects on direct and indirect tautomerism of pyrimidin-2(1H)-one/pyrimidin-2-ol. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, . | 0.9 | 0 |
| 17185 | Catalytic asymmetric C-H insertion reactions of vinyl carbocations. <i>Science</i> , 2022, 378, 1085-1091. | 6.0 | 19 |
| 17186 | Diantimony Complexes [$Cp^*_2Mo_2(CO)_4(\eta^4-\eta^2-\eta^2)$] ($Cp^*_2Mo_2(CO)_4(\eta^4-\eta^2-\eta^2)$) ($Cp^*_2Mo_2(CO)_4(\eta^4-\eta^2-\eta^2)$) as Unexpected Ligands Stabilizing Silver(I) ($n=1$) Monomers, Dimers and Chains. <i>Angewandte Chemie - International Edition</i> , 2023, 62, . | 7.2 | 3 |
| 17187 | Spectral features of the ferrous-CO complex in cytochrome P450: a revisit using TDDFT calculations. <i>Journal of Biological Inorganic Chemistry</i> , 2023, 28, 57-64. | 1.1 | 1 |
| 17188 | Prediction model on hydrolysis kinetics of phthalate monoester: A density functional theory study. <i>Journal of Environmental Sciences</i> , 2024, 135, 51-58. | 3.2 | 1 |
| 17189 | A Theoretical Study of Structural, Electronic, and Vibration Properties of Acetylcholine Chloride and Bromide. <i>Food Processing: Techniques and Technology</i> , 2022, 52, 718-728. | 0.3 | 0 |
| 17190 | Pump-probe spectroscopy of chiral vibrational dynamics. <i>Science Advances</i> , 2022, 8, . | 4.7 | 5 |
| 17191 | On the Quantum Confinement Effects in Ultrathin PdO Films by Experiment and Theory. <i>Materials</i> , 2022, 15, 8700. | 1.3 | 1 |
| 17192 | MoBioTools : A toolkit to setup quantum mechanics/molecular mechanics calculations. <i>Journal of Computational Chemistry</i> , 0, , . | 1.5 | 7 |
| 17193 | Behavior of HF and (HF) ₂ inside a fullerene cage: An in silico study using different density functionals. <i>International Journal of Quantum Chemistry</i> , 0, , . | 1.0 | 1 |
| 17194 | $\tilde{\rho}$ B97X-3c: A composite range-separated hybrid DFT method with a molecule-optimized polarized valence double- ζ basis set. <i>Journal of Chemical Physics</i> , 2023, 158, . | 1.2 | 18 |
| 17195 | Structural Investigation of DHICA Eumelanin Using Density Functional Theory and Classical Molecular Dynamics Simulations. <i>Molecules</i> , 2022, 27, 8417. | 1.7 | 0 |
| 17196 | Chain Walking in the $AlCl_3$ -Catalyzed Cationic Polymerization of \pm -Olefins. <i>ChemPlusChem</i> , 2023, 88, . | 1.3 | 5 |
| 17197 | Intercited State Photophysics I: Benchmarking Density Functionals for Computing Nonadiabatic Couplings and Internal Conversion Rate Constants. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 271-292. | 2.3 | 5 |
| 17198 | Molecular Design and Crystal Chemistry of Polyfluorinated Naphthalene-bis-phenylhydrazimides with Superior Thermal and Polymorphic Stability and High Solution Processability. <i>Chemistry - A European Journal</i> , 0, , . | 1.7 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 17199 | Quantum Chemical Prediction of the Acidities of Sulfonamide Inhibitors of Carbonic Anhydrase. <i>Journal of Physical Chemistry A</i> , 2022, 126, 9207-9217. | 1.1 | 2 |
| 17200 | Identification of potential inhibitors of omicron variant of SARS-Cov-2 RBD based virtual screening, MD simulation, and DFT. <i>Frontiers in Chemistry</i> , 0, 10, . | 1.8 | 1 |
| 17201 | Reactions of Thorium Oxide Clusters with Water: the Effects of Oxygen Content. <i>ChemPhysChem</i> , 0, , . | 1.0 | 0 |
| 17202 | Rare earth cerium-phenanthroline binary complex as a new corrosion inhibitor for carbon steel in acidic medium. <i>Research on Chemical Intermediates</i> , 2023, 49, 1235-1257. | 1.3 | 3 |
| 17203 | URVA and Local Mode Analysis of an Iridium Pincer Complex Efficiently Catalyzing the Hydrogenation of Carbon Dioxide. <i>Inorganics</i> , 2022, 10, 234. | 1.2 | 1 |
| 17204 | Prediction models of the ionization coefficient and ionization cross-section based on multi-layer molecular parameters. <i>Plasma Science and Technology</i> , 0, , . | 0.7 | 0 |
| 17205 | Visible Light-Induced Coupling Cyclization Reaction of $\hat{\pm}$ -Diazosulfonium Triflates with $\hat{\pm}$ -Oxocarboxylic Acids or Alkynes. <i>Journal of Organic Chemistry</i> , 2022, 87, 16604-16616. | 1.7 | 8 |
| 17206 | Ag decorated sea urchin-MoO ₃ based hierarchical micro-nano structures as surface - enhanced Raman spectroscopy substrates for the detection of a nitrosamine industrial pollutant. <i>Materials Today Communications</i> , 2022, 33, 104995. | 0.9 | 3 |
| 17207 | Investigating the Heaviest Halogen: Lessons Learned from Modeling the Electronic Structure of Astatine TM s Small Molecules. <i>Journal of Physical Chemistry A</i> , 2023, 127, 46-56. | 1.1 | 4 |
| 17208 | Exploration of the mechanism of the condensation reaction of Al(OH) ₄ ⁻ with a D-gluconate using density functional theory. <i>Structural Chemistry</i> , 0, , . | 1.0 | 0 |
| 17209 | Reaction of OH with Aliphatic and Aromatic Isocyanates. <i>Journal of Physical Chemistry A</i> , 2022, 126, 9333-9352. | 1.1 | 4 |
| 17210 | Insight into Stereocontrol in the Asymmetric Intramolecular Allylation with a <i>tert</i> -Butylsulfonamide Nucleophile: Application in the Synthesis of Chiral Isoindoline-1-Carboxylic Acid Esters. <i>Journal of Organic Chemistry</i> , 2023, 88, 613-625. | 1.7 | 2 |
| 17211 | The subsystem quantum chemistry program <scp>Serenity</scp>. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2023, 13, . | 6.2 | 11 |
| 17212 | Rotational Isomerization of Carbon ¹³ -Carbon Single Bonds in Ethyl Radical Derivatives in a Room-Temperature Solution. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 11551-11557. | 2.1 | 1 |
| 17213 | Andrographolide-based potential anti-inflammatory transcription inhibitors against nuclear factor NF- κ B p50 subunit (NF- κ B p50): an integrated molecular and quantum mechanical approach. <i>3 Biotech</i> , 2023, 13, . | 1.1 | 1 |
| 17214 | Electronic Structure and Magnetic Properties of a High ^{Spin} Mn ^{III} Complex: [Mn(mesacac) ₃] (mesacac=1,3 ⁻ Bis(2,4,6 ⁻ trimethylphenyl) ⁻ propane ^{-1,3} ⁻ dionato). <i>ChemPhysChem</i> , 0, , . | 1.0 | 1 |
| 17215 | Virtual Screening of Telaprevir and Danoprevir Derivatives for Hepatitis C Virus NS3/4A Protease Inhibitors. <i>Letters in Drug Design and Discovery</i> , 2024, 21, 809-822. | 0.4 | 0 |
| 17216 | N-Functionalization of 5-Aminotetrazoles: Balancing Energetic Performance and Molecular Stability by Introducing ADNP. <i>International Journal of Molecular Sciences</i> , 2022, 23, 15841. | 1.8 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17218 | A transferable recommender approach for selecting the best density functional approximations in chemical discovery. <i>Nature Computational Science</i> , 2023, 3, 38-47. | 3.8 | 10 |
| 17219 | A spur to molecular geometry optimization: Gradient-enhanced universal kriging with on-the-fly adaptive <i>ab initio</i> prior mean functions in curvilinear coordinates. <i>Journal of Chemical Physics</i> , 2023, 158, . | 1.2 | 4 |
| 17220 | Conferols A and B from the stems of <i>Dracaena conferta</i> Ridl.. <i>Tetrahedron</i> , 2023, 131, 133232. | 1.0 | 1 |
| 17221 | Die Diantimonkomplexe [Cp ² Mo ₂ (CO) ₄ (η^4 , η^2 -Sb ₂)] (Cp ² =C ₅ H ₅ , C ₅ H ₄ t ^{Bu}) als unerwartete stabilisierende Liganden von Silber(I) (<i>n</i> =1) Monomeren, μ -Dimeren und μ -Ketten. <i>Angewandte Chemie</i> , 2023, 135, . | 1.6 | 2 |
| 17222 | The dominant nature of Herzbergâ€Teller terms in the photophysical description of naphthalene compared to anthracene and tetracene. <i>Scientific Reports</i> , 2022, 12, . | 1.6 | 4 |
| 17223 | Computational Study of Iron-Catalyzed Intramolecular [2 + 2] Cycloaddition and Cycloisomerization of Enyne Acetates: Mechanism and Selectivity. <i>Journal of Organic Chemistry</i> , 2023, 88, 944-951. | 1.7 | 0 |
| 17224 | Design and biological activity of a novel fungicide, quinofumelin. <i>Journal of Pesticide Sciences</i> , 2023, , . | 0.8 | 0 |
| 17225 | Luminescent Metal-Organic Framework with 2,1,3-Benzothiadiazole Units for Highly Sensitive Gossypol Sensing. <i>Chemosensors</i> , 2023, 11, 52. | 1.8 | 6 |
| 17226 | Specific zinc binding to heliorhodopsin. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 3535-3543. | 1.3 | 8 |
| 17227 | The El-Sayedâ€™s rule analogy enables long-lived room temperature phosphorescence in twisted biphenyls. <i>Cell Reports Physical Science</i> , 2023, 4, 101245. | 2.8 | 10 |
| 17228 | Molecular Modelling of Ionic Liquids: Situations When Charge Scaling Seems Insufficient. <i>Molecules</i> , 2023, 28, 800. | 1.7 | 5 |
| 17229 | Modeling coarse-grained van der Waals interactions using dipole-coupled anisotropic quantum Drude oscillators. <i>Journal of Computational Chemistry</i> , 2023, 44, 1164-1173. | 1.5 | 1 |
| 17230 | Screening Carbonâ€“Boron Frustrated Lewis Pairs for Small-Molecule Activation including N ₂ , O ₂ , CO, CO ₂ , CS ₂ , H ₂ O and CH ₄ : A Computational Study. <i>Chemistry - an Asian Journal</i> , 2023, 18, . | 1.7 | 5 |
| 17231 | Nature-Derived Epoxy Resin Monomers with Reduced Sensitizing Capacityâ€”Elsorbide-Based Bis-Epoxides. <i>Chemical Research in Toxicology</i> , 2023, 36, 281-290. | 1.7 | 1 |
| 17232 | Synthesis and lewis acidity of fluorinated triaryl borates. <i>Dalton Transactions</i> , 2023, 52, 1820-1825. | 1.6 | 3 |
| 17233 | Structural, Electronic, and UV-Vis Properties for Cd _{11-n} Zn _n Te ₁₁ with (n = 0,2â€“5,11) Nanostructures: A DFT and TDDFT Study. <i>Journal of Electronic Materials</i> , 2023, 52, 2193-2200. | 1.0 | 1 |
| 17234 | Active Thermochemical Tables: Enthalpies of Formation of Bromo- and Iodo-Methanes, Ethenes and Ethynes. <i>Journal of Physical Chemistry A</i> , 2023, 127, 704-723. | 1.1 | 2 |
| 17235 | Direct detection of a single [4Feâ€“4S] cluster in a tungsten-containing enzyme: Electrochemical conversion of CO ₂ into formate by formate dehydrogenase. , 2023, 5, . | | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 17236 | Understanding Density-Driven Errors for Reaction Barrier Heights. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 532-543. | 2.3 | 11 |
| 17237 | Ionization energies of metallocenes: A coupled cluster study of cobaltocene. <i>Physical Chemistry Chemical Physics</i> , 0, , . | 1.3 | 3 |
| 17238 | Reactions $O(^3P, ^1D) + HCCN(X^1\Sigma^+)$ (Cyanoacetylene): Crossed-Beam and Theoretical Studies and Implications for the Chemistry of Extraterrestrial Environments. <i>Journal of Physical Chemistry A</i> , 2023, 127, 685-703. | 1.1 | 3 |
| 17239 | Benchmarking two-body contributions to crystal lattice energies and a range-dependent assessment of approximate methods. <i>Journal of Chemical Physics</i> , 2023, 158, . | 1.2 | 2 |
| 17240 | Nickel-catalysed regio- and stereoselective acylzincation of unsaturated hydrocarbons with organozincs and CO. , 0, , . | | 3 |
| 17241 | Stable fast-charging sodium-ion batteries achieved by a carbomethoxy-modified disodium organic material. <i>Cell Reports Physical Science</i> , 2023, , 101240. | 2.8 | 2 |
| 17242 | Photocatalytic Activity of the V2O5 Catalyst toward Selected Pharmaceuticals and Their Mixture: Influence of the Molecular Structure on the Efficiency of the Process. <i>Molecules</i> , 2023, 28, 655. | 1.7 | 4 |
| 17243 | Rational Design of Polymethine Dyes with NIR Emission and High Photothermal Conversion Efficiency for Multimodal Imaging-Guided Photothermal Immunotherapy. <i>Advanced Materials</i> , 2023, 35, . | 11.1 | 23 |
| 17244 | Low-cost machine learning prediction of excited state properties of iridium-centered phosphors. <i>Chemical Science</i> , 2023, 14, 1419-1433. | 3.7 | 6 |
| 17246 | Automatic purpose-driven basis set truncation for time-dependent Hartree-Fock and density-functional theory. <i>Nature Communications</i> , 2023, 14, . | 5.8 | 1 |
| 17247 | Asymmetric synthesis of complex tricyclo[3.2.2.0]nonenes from racemic norcaradienes: kinetic resolution via Diels-Alder reaction. <i>Chemical Science</i> , 2023, 14, 1844-1851. | 3.7 | 1 |
| 17248 | Electron Transfer Rates in Solution: Toward a Predictive First Principle Approach. <i>Chemistry</i> , 2023, 5, 97-105. | 0.9 | 1 |
| 17249 | Poly(ionic liquid)s for Photo-Driven CO ₂ Cycloaddition: Electron Donor-Acceptor Segments Matter. <i>Advanced Science</i> , 2023, 10, . | 5.6 | 10 |
| 17250 | Pyridine Dimers and Their Low-Temperature Isomerization: A High-Resolution Matrix Isolation Spectroscopy Study. <i>Angewandte Chemie</i> , 2023, 135, . | 1.6 | 0 |
| 17251 | Synthesis of new trisubstituted hexahydro-isoindole-1,3-dione derivatives regio- and stereoselectivity: spectroscopic and theoretical studies. <i>Chemical Papers</i> , 0, , . | 1.0 | 0 |
| 17252 | Atomistic insight into the effects of electrostatic fields on hydrocarbon reaction kinetics. <i>Journal of Chemical Physics</i> , 2023, 158, . | 1.2 | 1 |
| 17253 | First-principles evaluation of the second harmonic generation response of reference organic and inorganic crystals. <i>Journal of Chemical Physics</i> , 2023, 158, . | 1.2 | 2 |
| 17254 | Ab Initio Investigation of the Na ₃ [Ln(ODA) ₃] \cdot 2NaClO ₄ \cdot 6H ₂ O (Ln = Ce, Yb; ODA =) Tj EIQq1 1 0784314 | | |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17255 | Exciton dispersion and exciton-phonon interaction in solids by time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2023, 158, . | 1.2 | 0 |
| 17256 | Computational Insights into the Iron-Catalyzed Magnesium-Mediated Hydroformylation of Alkynes. <i>Journal of Organometallic Chemistry</i> , 2023, , 122621. | 0.8 | 2 |
| 17257 | Mechanistic Insights into the Reactive Uptake of Chlorine Nitrate at the Air-Water Interface. <i>Journal of the American Chemical Society</i> , 2023, 145, 944-952. | 6.6 | 3 |
| 17258 | Temperature, pressure, and adsorption dependent redox potentials: III. Processes of CO conversion to value-added compounds. <i>Energy Science and Engineering</i> , 2024, 12, 362-393. | 1.9 | 0 |
| 17259 | Effects of MOF linker rotation and functionalization on methane uptake and diffusion. <i>Molecular Systems Design and Engineering</i> , 2023, 8, 527-537. | 1.7 | 1 |
| 17260 | Computational methods and points for attention in absolute configuration determination. , 0, 1, . | | 9 |
| 17261 | Kinetic Modeling of a Poly(<i>N</i> -vinylcaprolactam- <i>co</i> -glycidyl methacrylate) Microgel Synthesis: A Hybrid In Silico and Experimental Approach. <i>Industrial & Engineering Chemistry Research</i> , 2023, 62, 893-902. | 1.8 | 5 |
| 17262 | Mechanism and Selectivity of Electrochemical Reduction of CO ₂ on Metalloporphyrin Catalysts from DFT Studies. <i>Molecules</i> , 2023, 28, 375. | 1.7 | 1 |
| 17263 | One-electron self-interaction error and its relationship to geometry and higher orbital occupation. <i>Journal of Chemical Physics</i> , 2023, 158, . | 1.2 | 5 |
| 17264 | Multifunctional Electrolyte Additive Enables Highly Reversible Anodes and Enhanced Stable Cathodes for Aqueous Zinc-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 4152-4165. | 4.0 | 8 |
| 17265 | Enzyme-independent catabolism of cysteine with pyridoxal-5-phosphate. <i>Scientific Reports</i> , 2023, 13, . | 1.6 | 2 |
| 17266 | Synthesis and DNase I Inhibitory Properties of New Squaramides. <i>Molecules</i> , 2023, 28, 538. | 1.7 | 1 |
| 17267 | Pyridine Dimers and Their Low-Temperature Isomerization: A High-Resolution Matrix Isolation Spectroscopy Study. <i>Angewandte Chemie - International Edition</i> , 2023, 62, . | 7.2 | 3 |
| 17268 | The change of hydrogen position on π -conjugated bridge to affect NLO property of D(NH ₂)-A(NO ₂) system. <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 114004. | 1.1 | 2 |
| 17269 | QM/MM study of N501 involved intermolecular interaction between SARS-CoV-2 receptor binding domain and antibody of human origin. <i>Computational Biology and Chemistry</i> , 2023, 102, 107810. | 1.1 | 0 |
| 17270 | Organic ligands activate the dark formation of hydroxyl radicals (HO•) in surface soil/sediment: Yields, mechanisms, and applications. <i>Journal of Hazardous Materials</i> , 2023, 446, 130710. | 6.5 | 3 |
| 17271 | Two birds with one stone: Cobalt-doping induces to enhanced piezoelectric property and persulfate activation ability of ZnO nanorods for efficient water purification. <i>Nano Energy</i> , 2023, 107, 108173. | 8.2 | 28 |
| 17272 | Effective ammonia separation by non-chloride deep eutectic solvents composed of dihydroxybenzoic acids and ethylene glycol through multiple-site interaction. <i>Separation and Purification Technology</i> , 2023, 309, 123136. | 3.9 | 14 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17273 | Promoting intense mechanoluminescence by strengthening C-H \cdots N interactions in thioxanthene derivatives. <i>Dyes and Pigments</i> , 2023, 211, 111054. | 2.0 | 3 |
| 17274 | Spectral studies, crystal structures, DNA binding, and anticancer potentials of Pd(II) complexes with iminophosphine ligands: Experimental and computational methods. <i>Inorganica Chimica Acta</i> , 2023, 547, 121368. | 1.2 | 3 |
| 17275 | Insights into the HCl formation and volatilization mechanism from organochlorine in coal: A DFT study. <i>Fuel</i> , 2023, 338, 127271. | 3.4 | 6 |
| 17276 | Molecular and Aggregate Structural, Thermal, Mechanical and Photophysical Properties of Long-Chain Amide Gelators Containing an $\hat{\pi}$ -Diketo Group in the Presence or Absence of a Tertiary Amine Group. <i>Gels</i> , 2023, 9, 36. | 2.1 | 0 |
| 17277 | N-Annulation of the BTI Rylene Imide Organic Building Block: Impact on the Optoelectronic Properties of $\hat{\pi}$ -Extended Molecular Structures. <i>Colorants</i> , 2023, 2, 22-30. | 0.9 | 1 |
| 17278 | The Peroxymonocarbonate Anion HCO ₄ ⁻ as an Effective Oxidant in the Gas Phase: A Mass Spectrometric and Theoretical Study on the Reaction with SO ₂ . <i>Molecules</i> , 2023, 28, 132. | 1.7 | 1 |
| 17279 | In-Situ Photoelectron Spectroscopy Investigation of Sulfurization-Induced Sodiophilic Sites with Model Systems of $\hat{\pi}$ -sexithiophene and p-sexiphenyl. <i>Batteries</i> , 2023, 9, 21. | 2.1 | 1 |
| 17280 | Asymmetric Catalytic Conjugate Addition of Cyanide to Chromones and $\hat{\pi}$ -Substituted Cyclohexenones. <i>ACS Catalysis</i> , 2023, 13, 877-886. | 5.5 | 7 |
| 17281 | Molecular modelling framework of metal-organic clusters for conserving surfaces: Langmuir sorption through the TD-DFT/ONIOM approach. <i>Molecular Simulation</i> , 2023, 49, 365-376. | 0.9 | 17 |
| 17282 | Theoretical Strategies for Functionalisation and Encapsulation of Nanotubes. , 2011, , 225-278. | | 0 |
| 17283 | Einseitige Borat $\hat{\pi}$ -Veresterung w \hat{A} hrend enzymatischer Nukleosid $\hat{\pi}$ -phosphorolyse: Scheinbare Gleichgewichtsverschiebungen und kinetische Auswirkungen**. <i>Angewandte Chemie</i> , 2023, 135, . | 1.6 | 0 |
| 17284 | Is explicitly correlated double hybrid DFT advantageous for vibrational frequencies?. <i>Canadian Journal of Chemistry</i> , 0, , . | 0.6 | 1 |
| 17285 | Intramolecular Diels $\hat{\pi}$ -Alder Reaction of a Biphenyl Group in a Strained <i>meta</i> -Quaterphenylene Acetylene. <i>Journal of Organic Chemistry</i> , 0, , . | 1.7 | 1 |
| 17286 | Mechanistic Study of Chemoselectivity for Carbon Radical Hydroxylation versus Chlorination with Fe ^{III} (OH)(Cl) Complexes. <i>Chemistry - an Asian Journal</i> , 2023, 18, . | 1.7 | 1 |
| 17287 | Experimental and computational insights into luminescence in atomically precise bimetallic Au ₆ Cu ₅ (MPA) ₅ ($\hat{\pi}$ = 0 $\hat{\pi}$ ²) clusters. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 9513-9521. | 1.3 | 4 |
| 17288 | Gas-phase formation and spectroscopic characterization of the disubstituted cyclopropenylidenes c-C ₃ (C ₂ H) ₂ , c-C ₃ (CN) ₂ , and c-C ₃ (C ₂ H)(CN). <i>Astronomy and Astrophysics</i> , 0, , . | 2.1 | 2 |
| 17289 | The Predictive Power of Exact Constraints and Appropriate Norms in Density Functional Theory. <i>Annual Review of Physical Chemistry</i> , 2023, 74, 193-218. | 4.8 | 22 |
| 17290 | Hydrogen-Atom Electronic Basis Sets for Multicomponent Quantum Chemistry. <i>ACS Omega</i> , 2023, 8, 5033-5041. | 1.6 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17291 | Predicting the structures and vibrational spectra of molecular crystals containing large molecules with the generalized energy-based fragmentation approach. <i>Journal of Chemical Physics</i> , 2023, 158, . | 1.2 | 6 |
| 17292 | A Non Expected Alternative Ni(0) Species in the Ni-Catalytic Aldehyde and Alcohol Arylation Reactions Facilitated by a 1,5-Diazaphosphacyclooctane Ligand. <i>Chemistry - A European Journal</i> , 2023, 29, . | 1.7 | 3 |
| 17293 | Surrogate Based Genetic Algorithm Method for Efficient Identification of Low-Energy Peptide Structures. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 1080-1097. | 2.3 | 2 |
| 17294 | Application of statistical learning and mechanistic modelling towards mapping the substrate electronic space in a Cu-catalyzed Suzuki-Miyaura coupling. <i>Catalysis Science and Technology</i> , 0, , . | 2.1 | 0 |
| 17295 | Enhancing effect of choline chloride-based deep eutectic solvents with polyols on the aqueous solubility of curcumin-insight from experiment and theoretical calculation. <i>Chinese Journal of Chemical Engineering</i> , 2023, 59, 160-168. | 1.7 | 1 |
| 17296 | Insights into the Reactivity of the Ring-Opening Reaction of Tetrahydrofuran by Intramolecular Group-13/P- and Al/Group-15-Based Frustrated Lewis Pairs. <i>ACS Omega</i> , 2023, 8, 5316-5331. | 1.6 | 2 |
| 17297 | A proton-assisted AIE active luminescent material having tunable emission in solution and solid state with anti-counterfeiting application: Smart high contrast on-off-on fluorescence switch. <i>New Journal of Chemistry</i> , 0, , . | 1.4 | 4 |
| 17298 | Interpolative Separable Density Fitting for Accelerating Two-Electron Integrals: A Theoretical Perspective. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 679-693. | 2.3 | 6 |
| 17299 | DFT Study of CuS-ZnS Heterostructures. <i>Minerals, Metals and Materials Series</i> , 2023, , 39-50. | 0.3 | 0 |
| 17300 | Effect of Dioldibenzoate Isomers as Electron Donors on the Performances of Ziegler-Natta Polypropylene Catalysts: Experiments and Calculations. <i>Journal of Physical Chemistry C</i> , 2023, 127, 2294-2302. | 1.5 | 2 |
| 17301 | Antimicrobial, Antiproliferative Effects and Docking Studies of Methoxy Group Enriched Coumarin-Chalcone Hybrids. <i>Chemistry and Biodiversity</i> , 2023, 20, . | 1.0 | 2 |
| 17302 | Mechanisms and energetics for hydrogen abstraction of thymine photosensitized by benzophenone from theoretical principles. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 6467-6472. | 1.3 | 2 |
| 17303 | Halogen-substituted salicylhydroximate copper(II) metallacrowns: from synthesis and structures to novel applications. <i>Mendeleev Communications</i> , 2023, 33, 37-40. | 0.6 | 1 |
| 17304 | $\text{XPu}(\text{CO})_n$ (X = B, Al, Ga; $n = 2$ to 4): π -Back-Bonding in Heterodinuclear Plutonium Boron Group Compounds with an End-On Carbonyl Ligand. <i>Journal of Physical Chemistry A</i> , 2023, 127, 1233-1243. | 1.1 | 1 |
| 17305 | Adsorption of Gd^{3+} in water by N, S Co-doped La-based metal organic frameworks: Experimental and theoretical calculation. <i>Journal of Solid State Chemistry</i> , 2023, 321, 123864. | 1.4 | 2 |
| 17306 | Assembly Rules and Dehydration Mechanism of an Unconventional Hydrate: On the Complexity of the Hydrates of Creatine Phosphate Sodium. <i>Crystal Growth and Design</i> , 0, , . | 1.4 | 1 |
| 17307 | The solvation of SOH group in hydrated HSO_4^- (H_2O) clusters. <i>Journal of Chemical Research</i> , 2023, 47, 174751982311539. | 0.6 | 0 |
| 17308 | Assessment of the Xenobiotics Toxicity Taking into Account Their Metabolism. <i>Computational Methods in Engineering & the Sciences</i> , 2023, , 21-51. | 0.3 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 17309 | Assigning ¹ H chemical shifts in paramagnetic mono- and bimetallic surface sites using DFT: a case study on the Union Carbide polymerization catalyst. <i>Chemical Science</i> , 0, , . | 3.7 | 0 |
| 17310 | Biased Borate Esterification during Nucleoside Phosphorylase-Catalyzed Reactions: Apparent Equilibrium Shifts and Kinetic Implications**. <i>Angewandte Chemie - International Edition</i> , 2023, 62, . | 7.2 | 1 |
| 17311 | A Reactive Molecular Dynamics Study of Chlorinated Organic Compounds. Part I: Force Field Development. <i>ChemPhysChem</i> , 2023, 24, . | 1.0 | 0 |
| 17312 | Noncollinear density functional theory. <i>Physical Review Research</i> , 2023, 5, . | 1.3 | 4 |
| 17313 | Curvature Effect in Polydimethylsiloxane Interaction with CO ₂ . Insights from Theory. <i>Journal of Physical Chemistry A</i> , 2023, 127, 876-885. | 1.1 | 0 |
| 17314 | Electronic structure and density functional theory. , 2023, , 3-35. | | 0 |
| 17315 | Understanding the Monomer Deuteration Effect on the Transition Temperature of poly(<i>N</i> -isopropylacrylamide) Microgels in H ₂ O. <i>Polymer Chemistry</i> , 0, , . | 1.9 | 1 |
| 17316 | On the concentration polarisation in molten Li salts and borate-based Li ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 0, , . | 1.3 | 1 |
| 17317 | A colorimetric and turn-on fluorescent sensor for cyanide and acetate-based Schiff base compound of 2,2-((1E,11E)-5,8-dioxa-2,11-diazadodeca-1,11-diene-1,12-diyl)bis(4-((E)-phenyldiazenyl)phenol). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 292, 122397. | 2.0 | 2 |
| 17318 | Elucidating l-tyrosine crystal phase transitions by Raman spectroscopy and ab initio calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2023, 176, 111234. | 1.9 | 1 |
| 17319 | Phenalenone derivatives: The voyage from photosensitizers to push-pull fluorescent molecules. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 439, 114587. | 2.0 | 1 |
| 17320 | Accurate cortisol detection in human saliva by an extended-gate-type organic transistor functionalized with a molecularly imprinted polymer. <i>Sensors and Actuators B: Chemical</i> , 2023, 382, 133458. | 4.0 | 9 |
| 17321 | Synthesis, characterization, in-vitro biological evaluation and theoretical studies of 1,2,3-triazoles derived from triclosan as difeniconazole analogues. <i>Journal of Molecular Structure</i> , 2023, 1280, 135053. | 1.8 | 3 |
| 17322 | Dissecting amide-I vibrations in histidine dipeptide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 292, 122424. | 2.0 | 0 |
| 17323 | Phenolic compounds extraction from propolis using imidazole-based ionic liquids: A theoretical and experimental study. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, . | 0.9 | 4 |
| 17324 | Interaction mechanisms of the binding of polychlorinated biphenyls to thyroid hormone transporters revealed based on quantum chemistry and spectroscopy. <i>Journal of Molecular Structure</i> , 2023, 1281, 135104. | 1.8 | 0 |
| 17325 | Branching ratios in the dissociative photoionization of iodomethane by photoelectron photoion coincidence. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 7383-7393. | 1.3 | 2 |
| 17326 | Calculation of electric field gradients in Cd(<i>scp</i>) model complexes of the CueR protein metal site. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 12277-12283. | 1.3 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 17327 | Stable Nitrogen-Centered Radicals with Anti-Kasha Emission. <i>Journal of Materials Chemistry C</i> , 0, , . | 2.7 | 3 |
| 17328 | Influence of stabilisers on the catalytic activity of supported Au colloidal nanoparticles for the liquid phase oxidation of glucose to glucaric acid: understanding the catalyst performance from NMR relaxation and computational studies. <i>Green Chemistry</i> , 2023, 25, 2640-2652. | 4.6 | 6 |
| 17329 | New nitrosyl ruthenium complexes with combined activities for multiple cardiovascular disorders. <i>Dalton Transactions</i> , 2023, 52, 5176-5191. | 1.6 | 2 |
| 17330 | Designing molecules with a high-spin (quintet, $S = 2$) ground state for magnetic and spintronic applications. <i>Molecular Systems Design and Engineering</i> , 2023, 8, 874-886. | 1.7 | 2 |
| 17331 | Magneto-structural studies on a number of doubly end-on cyanate and azide bridged dinuclear nickel(II) complexes with $\{N_3O\}$ donor Schiff base ligands. <i>RSC Advances</i> , 2023, 13, 11311-11323. | 1.7 | 1 |
| 17332 | Satellite ligand effects on magnetic exchange in dimers. A structural, magnetic and theoretical investigation of $Cu_2L_2X_4$ ($L =$ methylisothiazolinone and $X =$) | 1.0 | 1 |
| 17333 | Visualization Analysis of Weak Interactions in Chemical Systems. , 2024, , 240-264. | | 10 |
| 17334 | Accurate single crystal and gas-phase molecular structures of acenaphthene: a starting point in the search for the longest C-C bond. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 11464-11476. | 1.3 | 4 |
| 17335 | R2022: A DFT/MRCI Ansatz with Improved Performance for Double Excitations. <i>Journal of Physical Chemistry A</i> , 2023, 127, 2011-2025. | 1.1 | 5 |
| 17336 | Mechanical Interlocking Enhances the Electrocatalytic Oxygen Reduction Activity and Selectivity of Molecular Copper Complexes. <i>Journal of the American Chemical Society</i> , 2023, 145, 6087-6099. | 6.6 | 10 |
| 17337 | Spark Discharge Doping Achieving Unprecedented Control over Aggregate Fraction and Backbone Ordering in Poly(3-hexylthiophene) Solutions. <i>Small</i> , 2023, 19, . | 5.2 | 1 |
| 17338 | Discovery of novel anti-cyanobacterial allelochemicals by multi-conformational QSAR approach. <i>Aquatic Toxicology</i> , 2023, 256, 106420. | 1.9 | 2 |
| 17339 | A Concerted Redox and Light Activated Agent for Controlled Multimodal Therapy against Hypoxic Cancer Cells. <i>Advanced Materials</i> , 2023, 35, . | 11.1 | 8 |
| 17340 | Hydration study of Silymarin and its ethylene glycol derivatives compounds by Monte Carlo simulation method. <i>Structural Chemistry</i> , 0, , . | 1.0 | 1 |
| 17341 | Electronic structure theory on modeling short-range noncovalent interactions between amino acids. <i>Journal of Chemical Physics</i> , 2023, 158, 094301. | 1.2 | 0 |
| 17342 | Quadripartite bond length rule applied to two prototypical aromatic and antiaromatic molecules. <i>Journal of Molecular Modeling</i> , 2023, 29, . | 0.8 | 0 |
| 17343 | Cage Dynamics-Mediated High Ionic Transport in Li_2O Batteries with a Hybrid Aprotic Electrolyte: LiTFSI, Sulfolane, and N,N -Dimethylacetamide. <i>Journal of Physical Chemistry B</i> , 2023, 127, 2991-3000. | 1.2 | 0 |
| 17344 | Modeling the Photo-Absorption Properties of Noble Metal Nanoclusters: A Challenge for Density-Functional Theory. <i>Journal of Physical Chemistry C</i> , 2023, 127, 7718-7729. | 1.5 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17345 | Design of an Electrostatic Frequency Map for the NH Stretch of the Protein Backbone and Application to Chiral Sum Frequency Generation Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2023, 127, 2418-2429. | 1.2 | 3 |
| 17346 | Modelling of the torsional IR spectra of the HSSSH, DSSSH, and DSSSD molecules. <i>Computational and Theoretical Chemistry</i> , 2023, 1222, 114080. | 1.1 | 2 |
| 17347 | Computational Study of Driving Forces in ATSP, PDIQ, and P53 Peptide Binding: Câ•OÂ•Â•Câ•O Tetrel Bonding Interactions at Work. <i>Journal of Chemical Information and Modeling</i> , 0, , . | 2.5 | 0 |
| 17348 | Enhanced Fluorescence by Inter/Intramolecular Hydrogen Bonding in Si-Substituted Coumarins. <i>Journal of Physical Chemistry B</i> , 2023, 127, 3187-3196. | 1.2 | 2 |
| 17349 | The Importance of Solvent Effects in Calculations of NMR Coupling Constants at the Doubles Corrected Higher Random-Phase Approximation. <i>Magnetochemistry</i> , 2023, 9, 102. | 1.0 | 3 |
| 17350 | “Catalysis Made Asymmetric” Enantiomerization Catalysis Mediated by the Chiral System of a Perylene Bisimide Cyclophane. <i>Angewandte Chemie</i> , 2023, 135, . | 1.6 | 1 |
| 17351 | High sensitivity for detecting trace Sn ²⁺ in canned food using novel covalent organic frameworks. <i>Talanta</i> , 2023, 257, 124338. | 2.9 | 3 |
| 17352 | Revealing intrinsic changes of DNA induced by spore photoproduct lesion through computer simulation. <i>Biophysical Chemistry</i> , 2023, 296, 106992. | 1.5 | 0 |
| 17353 | Effect of SO ₂ on HCl removal over ethanol-hydrated CaO adsorbent: Mechanism of competitive adsorption and product layer shielding. <i>Chemical Engineering Journal</i> , 2023, 464, 142516. | 6.6 | 9 |
| 17354 | Modified viologen-assisted reversible bromine capture and release in flowless zinc-bromine batteries. <i>Chemical Engineering Journal</i> , 2023, 464, 142624. | 6.6 | 3 |
| 17355 | Development of thermally-stable NIR absorbing films based on heptamethine cyanine dyes with bistriflimide anion. <i>Progress in Organic Coatings</i> , 2023, 178, 107473. | 1.9 | 1 |
| 17356 | Unpaired electrons-induced geochemical activity of native sulfur in energy-triggered ring-opening process. <i>Geochimica Et Cosmochimica Acta</i> , 2023, 348, 355-368. | 1.6 | 0 |
| 17357 | Mechanisms and origins of stereoselectivity involved in NHC-catalyzed [3+3] Annulation of 2-bromoenals and β^2 -ketothioamides: A DFT study. <i>Molecular Catalysis</i> , 2023, 542, 113135. | 1.0 | 0 |
| 17358 | Dependence of predicted bulk properties of hexagonal hydroxyapatite on exchange correlation functional. <i>Computational Materials Science</i> , 2023, 224, 112153. | 1.4 | 5 |
| 17359 | Extraction and separation of Li ⁺ from high-ratio Mg/Li salt lake brines by [C2mim][NTf ₂] ionic liquid and a homemade extractor. <i>Desalination</i> , 2023, 553, 116450. | 4.0 | 7 |
| 17360 | Generation mechanism of singlet oxygen from the interaction of peroxymonosulfate and chloride in aqueous systems. <i>Water Research</i> , 2023, 235, 119904. | 5.3 | 34 |
| 17361 | Molecular modelling of ionic liquids: Perfluorinated anionic species with enlarged halogen substitutions. <i>Journal of Molecular Liquids</i> , 2023, 378, 121599. | 2.3 | 3 |
| 17362 | Theoretical study of the natural active structure of the Fe-SSZ-13 zeolite and its reactivity toward the methane to methanol oxidation reaction. <i>Chemical Physics Letters</i> , 2023, 819, 140440. | 1.2 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|------|-----------|
| 17363 | Biological determination, molecular docking and Hirshfeld surface analysis of rhodium(I)-N-heterocyclic carbene complex: Synthesis, crystal structure, DFT calculations, optical and non linear optical properties. <i>Inorganica Chimica Acta</i> , 2023, 551, 121459. | 1.2 | 3 |
| 17364 | Biphasic lignocellulose fractionation for staged production of cellulose nanofibers and reactive lignin nanospheres: A comparative study on their microstructures and effects as chitosan film reinforcing. <i>Chemical Engineering Journal</i> , 2023, 465, 142881. | 6.6 | 14 |
| 17365 | Ionic mononuclear [Fe] and heterodinuclear [Fe,Ru] bis(diphenylphosphino)alkane complexes: Synthesis, spectroscopy, DFT structures, cytotoxicity, and biomolecular interactions. <i>Journal of Inorganic Biochemistry</i> , 2023, 242, 112156. | 1.5 | 3 |
| 17366 | A copolyether with pendant cyclic carbonate segment for PEO-based solid polymer electrolyte. <i>Journal of Power Sources</i> , 2023, 570, 233049. | 4.0 | 4 |
| 17367 | Hydrogen bonding to graphene surface: A comparative computational study. <i>Inorganica Chimica Acta</i> , 2023, 551, 121454. | 1.2 | 0 |
| 17368 | Dual-reaction center catalyst based on common metals Cu-Mg-Al for synergistic peroxydisulfate adsorption-activation in Fenton-like process. <i>Applied Catalysis B: Environmental</i> , 2023, 327, 122468. | 10.8 | 20 |
| 17369 | Green synthesis and characterization of water soluble nanocarnosine: A prospective drug delivery system. <i>Applied Materials Today</i> , 2023, 32, 101812. | 2.3 | 0 |
| 17370 | The mechanism of carcinogenic heavy metal adsorption on a new monolayer AlP5. <i>Applied Surface Science</i> , 2023, 623, 157025. | 3.1 | 1 |
| 17371 | In-depth DFT insights into the crucial role of hydrogen bonding network in CO ₂ fixation into propylene oxide promoted by Biomass-Derived deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2023, 380, 121737. | 2.3 | 4 |
| 17372 | Changes in arginine metabolism in advanced Alzheimer's patients: Experimental and theoretical analyses. <i>Journal of Molecular Structure</i> , 2023, 1282, 135254. | 1.8 | 2 |
| 17373 | The mechanism of easier desorption of Fe atoms on the (1 0 0) surface of LiFePO ₄ and FePO ₄ . <i>Chemical Physics</i> , 2023, 570, 111891. | 0.9 | 1 |
| 17374 | Luminescent furo[2,3-c]isoquinolines as fluorophores - Tuning the luminophore by donor substitution. <i>Dyes and Pigments</i> , 2023, 214, 111190. | 2.0 | 1 |
| 17375 | Sulfido-bridged 1,2-bis(diphenylphosphino)ethane (dppe) appended trinuclear nickel(II) clusters: Crystallographic and computational analyses. <i>Inorganica Chimica Acta</i> , 2023, 551, 121471. | 1.2 | 2 |
| 17376 | A novel Schiff base ligand and its metal complexes: Synthesis, characterization, theoretical calculations, catalase-like and catecholase-like enzymatic activities. <i>Journal of Molecular Liquids</i> , 2023, 380, 121636. | 2.3 | 4 |
| 17377 | Direct observation on argon tagging nitrobenzene radical anion in gas phase: Infrared photodissociation spectroscopy and theoretical calculation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 294, 122482. | 2.0 | 2 |
| 17378 | Vertical $\tilde{\nu}_C$ -extension of dibenzopentalene: A combined experimental and computational study of a phenanthreno-benzopentalene derivative. <i>Computational and Theoretical Chemistry</i> , 2023, 1224, 114113. | 1.1 | 0 |
| 17379 | DFT theoretical and experimental studies unraveling the structural and electronic properties of niobium doped calcium apatite ceramics. <i>Materials Today Communications</i> , 2023, 35, 105873. | 0.9 | 0 |
| 17380 | Synthesis of Carbazole-Substituted thiosemicarbazone and its Cu(II) Complex, DNA/Protein Binding, Cytotoxic, antiproliferative activities and molecular docking studies. <i>Inorganic Chemistry Communication</i> , 2023, 152, 110711. | 1.8 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 17381 | Exploring the structural, photophysical and optoelectronic properties of a diaryl heptanoid curcumin derivative and identification as a SARS-CoV-2 inhibitor. <i>Journal of Molecular Structure</i> , 2023, 1281, 135110. | 1.8 | 6 |
| 17382 | Ultra-low limit of luminescent detection of gossypol by terbium(III)-based metal-organic framework. <i>Journal of Hazardous Materials</i> , 2023, 452, 131289. | 6.5 | 7 |
| 17383 | A colorimetric and turn-on fluorescent sensor for rapid and selective detection of Fe ³⁺ ion based on azo compound of 4-((4-(dimethylamino) phenyl)diazanyl)-N-(pyridin-2-yl)benzamide. <i>Journal of Molecular Structure</i> , 2023, 1283, 135289. | 1.8 | 2 |
| 17384 | A novel C6-sulfonated celastrol analog as a tyrosinase and melanin inhibitor: Design, synthesis, biological evaluation and molecular simulation. <i>Journal of Molecular Structure</i> , 2023, 1283, 135288. | 1.8 | 3 |
| 17385 | Performance enhancement of catechin-graphene quantum dot nanocomposites functionalized with carboxyl and doped/decorated with boron towards dye-sensitized solar cell applications: DFT and TD-DFT calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2023, 121, 108427. | 1.3 | 5 |
| 17386 | Co nanoparticles modified N-doped carbon nanosheets array as a novel bifunctional photothermal membrane for simultaneous solar-driven interfacial water evaporation and persulfate mediating water purification. <i>Applied Catalysis B: Environmental</i> , 2023, 330, 122556. | 10.8 | 16 |
| 17387 | Molecular structure of Ru(II)/diphosphine/4,6-dimethyl-2-pyrimidinethiol complexes: A combined experimental and density functional theory study. <i>Journal of Molecular Structure</i> , 2023, 1282, 135234. | 1.8 | 0 |
| 17388 | Novel low-bandgap donor-acceptor thiophene-phenylene co-oligomers for light-emitting semiconductor devices. <i>Dyes and Pigments</i> , 2023, 215, 111256. | 2.0 | 0 |
| 17389 | G-C3N5 nanotube as a promising candidate for adsorption and inactivation of aflatoxin B1: A first-principles study. <i>Surfaces and Interfaces</i> , 2023, 38, 102868. | 1.5 | 0 |
| 17390 | Magnetic properties and pH-controlled reversible interconversion of μ -oxido into μ -hydroxido in oxo-carboxylato bridged iron(III) dimers: Theoretical and experimental insights. <i>Journal of Molecular Structure</i> , 2023, 1285, 135426. | 1.8 | 1 |
| 17391 | Electronic structure and detonation property prediction of pentazole derivatives: Aminopentazole, diaminopentazole cations, azopentazole, and 1,2-diazopentazole. <i>Journal of Molecular Structure</i> , 2023, 1285, 135420. | 1.8 | 5 |
| 17392 | Photoinduced charge transfer in push-pull pyrazoline-based chromophores – Relationship between molecular structure and photophysical, photovoltaic properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 296, 122643. | 2.0 | 1 |
| 17393 | Control of the fluorescence molecule 2-(2-hydroxyphenyl) benzothiazole derivatives by introducing electron-donating and withdrawing substituents groups. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 296, 122666. | 2.0 | 4 |
| 17394 | Aqueous-phase photo-oxidation of selected green leaf volatiles initiated by OH radicals: Products and atmospheric implications. <i>Science of the Total Environment</i> , 2023, 879, 162622. | 3.9 | 2 |
| 17395 | Insights into interaction mechanism between xanthan gum and galactomannan based on density functional theory and rheological properties. <i>Food Chemistry</i> , 2023, 418, 135990. | 4.2 | 3 |
| 17396 | Cu-loaded MOF-303 for iodine adsorption: The roles of Cu species and pyrazole ligands. <i>Applied Surface Science</i> , 2023, 619, 156819. | 3.1 | 9 |
| 17397 | Development and catalytic mechanism of ionic liquid catalysts for polyoxymethylene dimethyl ethers. <i>Chemical Physics Letters</i> , 2023, 822, 140471. | 1.2 | 2 |
| 17398 | An electronic structure investigation of excited state intramolecular proton transfer in amino-benzazole derivatives: Relative energies and electron density descriptors. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 441, 114738. | 2.0 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17399 | Ionizable lipids penetrate phospholipid bilayers with high phase transition temperatures: perspectives from free energy calculations. <i>Chemistry and Physics of Lipids</i> , 2023, 253, 105294. | 1.5 | 3 |
| 17400 | Standard molar enthalpy of sublimation of form I nicotinamide. <i>Journal of Chemical Thermodynamics</i> , 2023, 182, 107042. | 1.0 | 0 |
| 17402 | Characterizing excited states of single donor-acceptor molecule by high-resolution Raman images. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2023, 461, 128648. | 0.9 | 1 |
| 17403 | Efficiently predicting directional carrier mobilities in organic materials with the Boltzmann transport equation. <i>Journal of Chemical Physics</i> , 2023, 158, . | 1.2 | 2 |
| 17404 | Experimental and computational studies of silver(I) dibenzoylmethane-based complexes, interaction with DNA/RNA/BSA biomolecules, and in vitro cytotoxic activity. <i>Journal of Inorganic Biochemistry</i> , 2023, 241, 112132. | 1.5 | 3 |
| 17405 | Engineering the packing structure of thioether- and sulfone- substituted dibenzo[a,e]pentalenes by pentafluorophenyl substitution. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, . | 0.9 | 2 |
| 17406 | Controlling Near-Infrared Photoluminescence Properties of Single-Walled Carbon Nanotubes by Substituent Effect in Stepwise Chemical Functionalization. <i>Journal of Physical Chemistry C</i> , 2023, 127, 2360-2370. | 1.5 | 5 |
| 17407 | Computational Study on Chemoselective Difunctionalization of Unactivated Alkenes with Radical-mediated Remote Functional Group Migration. <i>ChemPhysChem</i> , 2023, 24, . | 1.0 | 1 |
| 17408 | High-temperature mid-IR absorption and reaction kinetics of 2-methyl-1,3-dioxolane: An experimental and theoretical study. <i>Journal of Photochemistry and Photobiology</i> , 2023, 13, 100165. | 1.1 | 2 |
| 17409 | Molecular encapsulation of bioactive ingredients from Xuefu Zhuyu decoction by cyclodextrin-assisted extraction. <i>Journal of Drug Delivery Science and Technology</i> , 2023, 81, 104219. | 1.4 | 0 |
| 17410 | Reaction profiles for quantum chemistry-computed [3+2] cycloaddition reactions. <i>Scientific Data</i> , 2023, 10, . | 2.4 | 5 |
| 17411 | Chlorinated Cubane-1,4-dicarboxylic Acids. <i>Journal of Organic Chemistry</i> , 0, , . | 1.7 | 1 |
| 17412 | Exact Two-Component TDDFT with Simple Two-Electron Picture-Change Corrections: X-ray Absorption Spectra Near L- and M-Edges of Four-Component Quality at Two-Component Cost. <i>Journal of Physical Chemistry A</i> , 2023, 127, 1360-1376. | 1.1 | 6 |
| 17413 | Pyrrrolizidine alkaloids from <i>Jacobaea vulgaris</i> Gaertn and theoretical studies on intramolecular interactions. <i>Natural Product Research</i> , 0, , 1-6. | 1.0 | 1 |
| 17414 | Synthesis, enzyme inhibition, and molecular docking studies of a novel chalcone series bearing benzothiazole scaffold. <i>Biotechnology and Applied Biochemistry</i> , 2023, 70, 1357-1370. | 1.4 | 2 |
| 17415 | Assessing the accuracy of hybrid exchange-correlation functionals for the density response of warm dense electrons. <i>Journal of Chemical Physics</i> , 2023, 158, . | 1.2 | 8 |
| 17416 | Exploring novel fluorine-rich fuberidazole derivatives as hypoxic cancer inhibitors: Design, synthesis, pharmacokinetics, molecular docking, and DFT evaluations. <i>PLoS ONE</i> , 2023, 18, e0262790. | 1.1 | 0 |
| 17417 | Multi-Hydration Induced Zwitterionic Hydrogel with Open Environment Stability for Chemical Sensing. , 2023, 2, . | | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 17418 | Exploring Coumarin-Based Boron Emissive Complexes as Temperature Thermometers in Polymer-Supported Materials. <i>Sensors</i> , 2023, 23, 1689. | 2.1 | 3 |
| 17419 | Structure of <i>Geobacter</i> cytochrome OmcZ identifies mechanism of nanowire assembly and conductivity. <i>Nature Microbiology</i> , 2023, 8, 284-298. | 5.9 | 27 |
| 17420 | Mechanistic Insights into Substrate Positioning That Distinguish Non-heme Fe(II)/ α -Ketoglutarate-Dependent Halogenases and Hydroxylases. <i>ACS Catalysis</i> , 2023, 13, 2489-2501. | 5.5 | 10 |
| 17421 | Alternative Strategy for Spectral Tuning of Flavin-Binding Fluorescent Proteins. <i>Journal of Physical Chemistry B</i> , 2023, 127, 1301-1311. | 1.2 | 4 |
| 17422 | Investigation of the Impact of High Concentration LiTFSI Electrolytes on Silicon Anodes with Reactive Force Field Simulations. <i>Liquids</i> , 2023, 3, 132-158. | 0.8 | 1 |
| 17423 | Thermal site energy fluctuations in photosystem I: new insights from MD/QM/MM calculations. <i>Chemical Science</i> , 2023, 14, 3117-3131. | 3.7 | 1 |
| 17424 | Theoretical exploration of polynitrogen compounds N_6 , N_8 , N_{10} , and N_6 ions based on N_3^+ and $cyclo-N_5^+$. <i>Journal of Energetic Materials</i> , 0, 1-19. | 1.0 | 3 |
| 17425 | Physical Chemistry in Context: Using Quantum Mechanics to Understand the Greenhouse Effect. <i>Journal of Chemical Education</i> , 2023, 100, 1333-1342. | 1.1 | 0 |
| 17426 | Exploring the influence of free radicals on photolytic removal of nadolol from water: Mechanism of degradation and toxicity of intermediates. <i>Frontiers in Environmental Science</i> , 0, 11, . | 1.5 | 1 |
| 17427 | Model Chemistry Recommendations for Scaled Harmonic Frequency Calculations: A Benchmark Study. <i>Journal of Physical Chemistry A</i> , 2023, 127, 1715-1735. | 1.1 | 19 |
| 17428 | Gefapixant Citrate (MK-7264) Sulfonamide Step Speciation Study: Investigation into Precipitation/Dissolution Events during Addition of Chlorosulfonic Acid. <i>Organic Process Research and Development</i> , 2023, 27, 286-294. | 1.3 | 2 |
| 17429 | Small, Electron-Donating Substituents Give CO_2 Activation by Permethylpentalene Zirconium Amido Complexes the Upper Hand: A DFT Study of Distortion and Interaction. <i>Inorganic Chemistry</i> , 2023, 62, 3000-3006. | 1.9 | 0 |
| 17430 | Theoretical Studies of Mutual Effects between α -Hemiketalization and β -Lactonization in Pimaricin Thioesterase. <i>Chemistry - an Asian Journal</i> , 2023, 18, . | 1.7 | 1 |
| 17431 | Unusual Square Pyramidal Chalcogenide Mo_5 Cluster with Bridging Pyrazolate-Ligands. <i>International Journal of Molecular Sciences</i> , 2023, 24, 3440. | 1.8 | 3 |
| 17432 | On the self-consistency of DFT-1/2. <i>Journal of Chemical Physics</i> , 2023, 158, . | 1.2 | 0 |
| 17433 | Local Reactivity on Carbon Quantum Dots: The Influence of the Geometries and Chemical Doping for Chemical Sensor Applications. <i>Journal of Physical Chemistry C</i> , 2023, 127, 3819-3829. | 1.5 | 2 |
| 17434 | Ph_2Te_2 : An Accessible Main Group Organometallic Target for Spectral Characterization and Modeling. <i>Journal of Chemical Education</i> , 2023, 100, 1313-1319. | 1.1 | 0 |
| 17435 | Doping of Graphene Nanostructure with Iron, Nickel and Zinc as Selective Detector for the Toxic Gas Removal: A Density Functional Theory Study. <i>Journal of Carbon Research</i> , 2023, 9, 20. | 1.4 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17436 | Schiff Bases and Stereocontrolled Formation of Fused 1,3-Oxazolidines from 1-Amino-2-Indanol: A Systematic Study on Structure and Mechanism. <i>Molecules</i> , 2023, 28, 1670. | 1.7 | 1 |
| 17437 | The Selection of the Best Derivatization Reagents for the Determination of Polyamines in Home-Made Wine Samples. <i>Materials</i> , 2023, 16, 1474. | 1.3 | 3 |
| 17438 | Solvent-Mediated Tunable Regiodivergent C6- and N1-Alkylations of 2,3-Disubstituted Indoles with <i>p</i> -Quinone Methides. <i>Journal of Organic Chemistry</i> , 2023, 88, 3132-3147. | 1.7 | 1 |
| 17439 | Enhancing cation storage performance of layered double hydroxides by increasing the interlayer distance. <i>Journal of Chemical Physics</i> , 2023, 158, 094703. | 1.2 | 1 |
| 17440 | Naphthalene Phthalimide Derivatives as Model Compounds for Electrochromic Materials. <i>Molecules</i> , 2023, 28, 1740. | 1.7 | 3 |
| 17441 | Extending density functional theory with near chemical accuracy beyond pure water. <i>Nature Communications</i> , 2023, 14, . | 5.8 | 7 |
| 17442 | Heteropolymetallic [FeFe]-Hydrogenase Mimics: Synthesis and Electrochemical Properties. <i>Inorganic Chemistry</i> , 2023, 62, 3409-3419. | 1.9 | 1 |
| 17443 | <i>Operando</i> characterization of rhodium catalyst degradation in hydroformylation. <i>Catalysis Science and Technology</i> , 2023, 13, 1788-1801. | 2.1 | 3 |
| 17444 | BODIPY-Based Photothermal Agents with Excellent Phototoxic Indices for Cancer Treatment. <i>Journal of the American Chemical Society</i> , 2023, 145, 4534-4544. | 6.6 | 18 |
| 17445 | A localized high concentration carboxylic ester-based electrolyte for high-voltage and low temperature lithium batteries. <i>Chemical Engineering Journal</i> , 2023, 461, 141904. | 6.6 | 7 |
| 17446 | The CO ₂ Reduction Reaction Mechanism on Silicene Nanoflakes. A Theoretical Perspective. <i>ChemistrySelect</i> , 2023, 8, . | 0.7 | 5 |
| 17447 | Machine Learning-Guided Computational Screening of New Candidate Reactions with High Bioorthogonal Click Potential. <i>Chemistry - A European Journal</i> , 0, , . | 1.7 | 6 |
| 17448 | P-Stereogenic Ir-MaxPHOX: A Step toward Privileged Catalysts for Asymmetric Hydrogenation of Nonchelating Olefins. <i>ACS Catalysis</i> , 2023, 13, 3020-3035. | 5.5 | 11 |
| 17449 | Interactions of Sodium Salicylate with β -Cyclodextrin and an Anionic Resorcin[4]arene: Mutual Diffusion Coefficients and Computational Study. <i>International Journal of Molecular Sciences</i> , 2023, 24, 3921. | 1.8 | 0 |
| 17450 | Quasiclassical Trajectory Simulation as a Protocol to Build Locally Accurate Machine Learning Potentials. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 1133-1142. | 2.5 | 1 |
| 17451 | Mechanistic insight into the ligand-controlled regioselective hydrocarboxylation of aryl olefins with palladium catalyst: A computational study. <i>Journal of Organometallic Chemistry</i> , 2023, 989, 122645. | 0.8 | 0 |
| 17452 | Porous and Stable Zn-Series Metal-Organic Frameworks as Efficient Catalysts for Grafting Wood Nanofibers with Polycaprolactone via a Copolymerization Approach. <i>Inorganic Chemistry</i> , 2023, 62, 3464-3473. | 1.9 | 5 |
| 17453 | Heterophenoquinones: Tuning Optoelectronics and Electrochromicity. <i>Chemistry - A European Journal</i> , 0, , . | 1.7 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17454 | Synthesis and the In Vitro Evaluation of Antitumor Activity of Novel Thiobenzanilides. <i>Molecules</i> , 2023, 28, 1877. | 1.7 | 0 |
| 17455 | Improving the TADF in Corannulene-Based Emitters via Tuning the Strength of Donor and Acceptor Groups. <i>Advanced Theory and Simulations</i> , 2023, 6, . | 1.3 | 0 |
| 17456 | Mechanisms for Catalytic CO Oxidation on SiAun (n = 1-5) Cluster. <i>Molecules</i> , 2023, 28, 1917. | 1.7 | 0 |
| 17457 | Deciphering the ground state of a C3-symmetrical Blatter-type triradical by CW and pulse EPR spectroscopy. <i>Journal of Magnetic Resonance</i> , 2023, 349, 107406. | 1.2 | 2 |
| 17458 | CO Inversion on a NaCl(100) Surface: A Multireference Quantum Embedding Study. <i>Journal of Physical Chemistry A</i> , 2023, 127, 1975-1987. | 1.1 | 2 |
| 17459 | Intrinsic Charge Transport for DTzTI-Based All-Acceptor Homopolymer n-Type Organic Semiconductors: Roles of Conjugation Length and Orbital Delocalization. <i>Journal of Physical Chemistry C</i> , 2023, 127, 4273-4282. | 1.5 | 2 |
| 17460 | Centrosymmetric Nickel(II) Complexes Derived from Bis-(Dithiocarbamato)piperazine with 1,1'-Bis-(Diphenylphosphino)ferrocene and 1,2-Bis-(Diphenylphosphino)ethane as Ancillary Ligands: Syntheses, Crystal Structure and Computational Studies. <i>Crystals</i> , 2023, 13, 343. | 1.0 | 2 |
| 17461 | Can Copper(I) and Silver(I) be Hydrogen Bond Acceptors?. <i>Chemistry - A European Journal</i> , 0, , . | 1.7 | 0 |
| 17462 | Effect of molecular weight on the properties of water-soluble terpolymers for heavy oil viscosity reduction. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2023, 144, 104738. | 2.7 | 6 |
| 17463 | Femtosecond Time-Resolved Observation of Relaxation and Wave Packet Dynamics of the S1 State in Electronically Excited o-Fluoroaniline. <i>Molecules</i> , 2023, 28, 1999. | 1.7 | 0 |
| 17464 | In-source fragmentation of nucleosides in electrospray ionization towards more sensitive and accurate nucleoside analysis. <i>Analyst</i> , 2023, 148, 1500-1506. | 1.7 | 1 |
| 17465 | Switchable Organic Low-Loss Spin Filters Based on Gold-Viologen-Gold Molecular Junctions. <i>Journal of Physical Chemistry C</i> , 2023, 127, 4251-4257. | 1.5 | 0 |
| 17466 | Oxygenated Boron Species Generated In Situ by Protonolysis Enables Precision Synthesis of Alternating Polyesters. <i>Macromolecules</i> , 2023, 56, 1907-1920. | 2.2 | 10 |
| 17467 | Carbonized Bacterial Cellulose-Derived Binder-Free, Flexible, and Free-Standing Cathode Host for High-Performance Stable Potassium-Sulfur Batteries. <i>ACS Applied Energy Materials</i> , 2023, 6, 3042-3051. | 2.5 | 7 |
| 17468 | Theoretical Study on the Catalytic CO ₂ Hydrogenation over the MOF-808-Encapsulated Single-Atom Metal Catalysts. <i>Journal of Physical Chemistry C</i> , 2023, 127, 4051-4062. | 1.5 | 3 |
| 17469 | Site of the Hydroxyl Group Determines the Surface Behavior of Bipolar Chain-Oxidized Cholesterol Derivatives: Langmuir Monolayer Studies Supplemented with Theoretical Calculations. <i>Journal of Physical Chemistry B</i> , 2023, 127, 2011-2021. | 1.2 | 4 |
| 17470 | Hierarchical Aggregation in a Complex Fluid: The Role of Isomeric Interconversion. <i>Journal of Physical Chemistry B</i> , 2023, 127, 2052-2065. | 1.2 | 0 |
| 17471 | Fluorinated Multi-Walled Carbon Nanotubes Coated Separator Mitigates Polysulfide Shuttle in Lithium-Sulfur Batteries. <i>Materials</i> , 2023, 16, 1804. | 1.3 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 17472 | Enhanced performance of Pd-[DBU][Cl]/AC mercury-free catalysts in acetylene hydrochlorination. Chinese Journal of Catalysis, 2023, 46, 137-147. | 6.9 | 1 |
| 17473 | Effects of Different Lengths of Oligo (Ethylene Glycol) Side Chains on the Electrochromic and Photovoltaic Properties of Benzothiadiazole-Based Donor-Acceptor Conjugated Polymers. Molecules, 2023, 28, 2056. | 1.7 | 4 |
| 17474 | DFT Studies on a Metal Oxide@Graphene-Decorated D ₁ -D ₂ -A Novel Multi-Junction Light-Harvesting System for Efficient Dye-Sensitized Solar Cell Applications. ACS Omega, 2023, 8, 8865-8875. | 1.6 | 0 |
| 17475 | Synthesis of a Novel Hydrazone of Thieno[2,3-d]pyrimidine Clubbed with Ninhydrin: X-ray Crystal Structure and Computational Investigations. Crystals, 2023, 13, 384. | 1.0 | 0 |
| 17476 | Fluorine-based Zn salan complexes. Dalton Transactions, 2023, 52, 4044-4057. | 1.6 | 1 |
| 17477 | Red-Fluorescing Paramagnetic Conjugated Polymer Nanoparticles ⁺ Triphenyl Methyl Radicals as Monomers in C-C Cross-Coupling Dispersion Polymerization. Macromolecules, 2023, 56, 2104-2112. | 2.2 | 3 |
| 17478 | A DFT Investigation of the Reactivity of Guanidinium Salts in Tandem aza-Michael Addition/Intramolecular Cyclization. Molecules, 2023, 28, 2218. | 1.7 | 1 |
| 17479 | Impact of External Electronic Perturbations on Single-Walled Carbon Nanotube Electronic Structure: Scanning Tunneling Spectroscopy and Density Functional Theory. Journal of Physical Chemistry C, 2023, 127, 4651-4659. | 1.5 | 2 |
| 17480 | Metal-coordinated polybenzimidazole membranes with preferential K ⁺ transport. Nature Communications, 2023, 14, . | 5.8 | 8 |
| 17481 | Comparisons of bpy and phen Ligand Backbones in Cr-Mediated (Co-)Electrocatalytic CO ₂ Reduction. Organometallics, 2023, 42, 1139-1148. | 1.1 | 2 |
| 17482 | Density Functional Theory Guided Investigation of Ligand-Induced Neptunyl-Neptunyl Interactions. European Journal of Inorganic Chemistry, 2023, 26, . | 1.0 | 2 |
| 17483 | A DFT study of Ni-catalyzed (3 + 3)-annulation between donor-acceptor cyclopropanes and diaziridines. Organic Chemistry Frontiers, 2023, 10, 1948-1958. | 2.3 | 4 |
| 17484 | Toward DMC Accuracy Across Chemical Space with Scalable \hat{T} -QML. Journal of Chemical Theory and Computation, 2023, 19, 1711-1721. | 2.3 | 4 |
| 17485 | Electron Spectroscopy of Charge Exchange Effects in Low Energy Ion Scattering at Surfaces: Case Studies of Heavy Ions at Al Surface. Surfaces, 2023, 6, 64-82. | 1.0 | 1 |
| 17486 | Light-induced infrared difference spectroscopy on three different forms of orange carotenoid protein: focus on carotenoid vibrations. Photochemical and Photobiological Sciences, 0, , . | 1.6 | 2 |
| 17487 | Extension of the TraPPE Force Field for Battery Electrolyte Solvents. Journal of Physical Chemistry B, 2023, 127, 2224-2236. | 1.2 | 1 |
| 17488 | Crystal-chemical characterisation and spectroscopy of fluorocarletonite and carletonite. Mineralogical Magazine, 2023, 87, 356-368. | 0.6 | 4 |
| 17490 | Dual Behavior Regulation: Tether-Free Deep-Brain Stimulation by Photothermal and Upconversion Hybrid Nanoparticles. Advanced Materials, 2023, 35, . | 11.1 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 17491 | Interface engineering of LDH-based material as efficient anti-corrosive system via synergetic performance of host, interlayers, and morphological features of nature-mimic architectures. <i>Chemical Engineering Journal</i> , 2023, 462, 142239. | 6.6 | 17 |
| 17492 | Electron heat transport in low-rank lignite: combining experimental and computational methods. <i>Journal of Thermal Analysis and Calorimetry</i> , 2023, 148, 4759-4768. | 2.0 | 3 |
| 17493 | Exploring electronic energy level structure and excited electronic states of β^2 -carotene using DFT. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 9373-9381. | 1.3 | 5 |
| 17494 | Mechanistic DFT Study of 1,3-Dipolar Cycloadditions of Azides with Guanidine. <i>Molecules</i> , 2023, 28, 2342. | 1.7 | 3 |
| 17495 | Exhaust Gases as Fluxing Agents for Palladium: Formation Enthalpies and Vapor Pressures of PdO, Pd ₂ (CO) _n ($n = 1-3$), Pd(NO) _n ($n = 1, 2$). <i>Journal of Physical Chemistry C</i> , 2023, 127, 4917-4933. | 1.5 | 1 |
| 17496 | Amide-Functional, Li ₃ N/Li-Rich Heterostructured Electrode Electrolyte Interphases for 4.6V Li LiCo ₂ Batteries. <i>Advanced Energy Materials</i> , 2023, 13, . | 10.2 | 31 |
| 17497 | Design, synthesis, molecular docking studies and biological evaluation of thiazole carboxamide derivatives as COX inhibitors. <i>BMC Chemistry</i> , 2023, 17, . | 1.6 | 8 |
| 17498 | Selective binding and periodic arrangement of magic boron clusters on monolayer borophene. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2023, 120, . | 3.3 | 2 |
| 17499 | Dual emission of ES IPT-capable 2-(2-hydroxyphenyl)-4-(1H-pyrazol-1-yl)pyrimidines: interplay of fluorescence and phosphorescence. <i>New Journal of Chemistry</i> , 2023, 47, 6361-6377. | 1.4 | 6 |
| 17500 | Solvation Effects on Polarizability of Aromatic Fluids. <i>Journal of Physical Chemistry B</i> , 2023, 127, 2237-2249. | 1.2 | 0 |
| 17501 | Mechanism and origins of ligand-controlled regioselectivity of copper-catalyzed borocarbonylation of imines with B ₂ pin ₂ and alkyl iodides: a computational study. <i>Organic Chemistry Frontiers</i> , 2023, 10, 2024-2032. | 2.3 | 0 |
| 17502 | Quest for singlet fission of organic sulfur-containing systems in the higher lying singlet excited state: application prospects of anti-Kasha's rule. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 9115-9122. | 1.3 | 0 |
| 17503 | Photoactivities of thiophene monomer/polymer transition in gel-based photoelectrochemical assembly: A theoretical/experimental approach. <i>International Journal of Electrochemical Science</i> , 2023, 18, 100077. | 0.5 | 0 |
| 17504 | Unraveling the charge transfer variation of tetrathiafulvalene-based organic crystals through fragment charge difference calculation. <i>APL Materials</i> , 2023, 11, 031104. | 2.2 | 0 |
| 17505 | Electrochemistry of Uranyl Peroxide Solutions during Electrospray Ionization. <i>Inorganic Chemistry</i> , 2023, 62, 4456-4466. | 1.9 | 4 |
| 17506 | TADF and X-ray Radioluminescence of New Cu(I) Halide Complexes: Different Halide Effects on These Processes. <i>International Journal of Molecular Sciences</i> , 2023, 24, 5145. | 1.8 | 2 |
| 17507 | Stability of sulfur molecules and insights into sulfur allotropy. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 9294-9299. | 1.3 | 4 |
| 17508 | Reactions of Zinc Hydride with Silylenes: From Oxidative Addition to Ligand Exchange Reactions. <i>Organometallics</i> , 2023, 42, 457-464. | 1.1 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17509 | Vanadium Pentafulvene Complexes: Synthon for Unprecedented Vanadocene^{III}Derivatives. Chemistry - A European Journal, 2023, 29, . | 1.7 | 1 |
| 17510 | Is DFT Accurate Enough to Calculate Regioselectivity? The Case of 1,3- Δ Dipolar Cycloaddition of Azide to Alkynes and Alkenes. ChemPhysChem, 2023, 24, . | 1.0 | 2 |
| 17511 | Multicomponent wavefunction-in-DFT embedding for positronium molecules. Journal of Chemical Physics, 2023, 158, . | 1.2 | 1 |
| 17512 | Density functional study on electrochemical reduction of carbon dioxide to C1 products using zinc oxide catalyst. Theoretical Chemistry Accounts, 2023, 142, . | 0.5 | 2 |
| 17513 | $\text{D}_2\text{D}_2\text{D}_2\text{D}^{\circ}\tilde{\text{N}},\tilde{\text{N}}\in\text{D}^{\circ}\text{D}\gg\tilde{\text{N}}\text{CED}1/2\tilde{\text{N}}-\tilde{\text{N}}\dots\text{D}^{\circ}\tilde{\text{N}}\in\text{D}^{\circ}\text{D}^{\circ}\tilde{\text{N}},\text{D}_\mu\tilde{\text{N}}\in\text{D},\tilde{\text{N}},\text{D},\text{D}^{\circ}\text{D},\text{D}_2\text{D}^{\circ}\tilde{\text{N}}\text{D},\text{D}^2\text{D}^3/4\text{D}^2\text{D}^{\circ}\text{D}1/2\text{D},\tilde{\text{N}}\dots\text{D}^{\circ}\text{D}^2\text{D}^{\circ}\text{D}1/2\tilde{\text{N}},\text{D}^3/4\text{D}^{\circ}\text{D},\tilde{\text{N}}\dots\tilde{\text{N}},\text{D}^3/4\tilde{\text{N}}\dagger\text{D}^3/4\text{D}^{\circ}\text{D}$ | | |
| 17514 | Ternary synergistic aggregation of chlorophyll/Soy protein isolate improves chlorophyll stability. Food Hydrocolloids, 2023, 140, 108662. | 5.6 | 1 |
| 17515 | “ $\text{C}^{\circ}\text{C}^{\circ}\text{C}^{\circ}$ Catalysis Made Asymmetric” Enantiomerization Catalysis Mediated by the Chiral $\text{C}^{\circ}\text{C}^{\circ}\text{C}^{\circ}$ System of a Perylene Bisimide Cyclophane. Angewandte Chemie - International Edition, 2023, 62, . | 7.2 | 5 |
| 17516 | Low-Temperature Observation of the Excited-State Decay of Ruthenium-(Mono-2,2,6,6-Terpyridine) Ions with Innocent Ligands: DFT Modeling of an $^3\text{MLCT}\rightarrow^3\text{MC}$ Intersystem Crossing Pathway. ACS Omega, 2023, 8, 11623-11633. | 1.6 | 1 |
| 17517 | Application of SnOx/AC catalyst for the acetylene hydrochlorination. Nano Research, 0, , . | 5.8 | 0 |
| 17518 | Target State Optimized Density Functional Theory for Electronic Excited and Diabatic States. Journal of Chemical Theory and Computation, 2023, 19, 1777-1789. | 2.3 | 3 |
| 17519 | Impact of active sites on encapsulation of curcumin in Metal Organic Frameworks. Materials Research Express, 2023, 10, 035102. | 0.8 | 3 |
| 17520 | Theoretical Research Methods Involved in This Book. Springer Theses, 2023, , 19-43. | 0.0 | 0 |
| 17521 | Characterizing the Impact of Mg-Doped Li Metal Anode and Excess Electrons on High Concentration Electrolyte Interfacial Stability: A Theoretical Study. ACS Applied Energy Materials, 2023, 6, 3291-3300. | 2.5 | 0 |
| 17522 | Finite element analysis on the near field properties of metallic cavities with atomic sharpness. Results in Physics, 2023, 47, 106360. | 2.0 | 0 |
| 17523 | Model selection in atomistic simulation. Journal of Chemical Physics, 2023, 158, . | 1.2 | 1 |
| 17524 | Nanostructured system based on hydroxyapatite and curcumin: A promising candidate for osteosarcoma therapy. Ceramics International, 2023, 49, 19932-19949. | 2.3 | 5 |
| 17525 | Influence of Rare-Earth Ion Radius on Metal-Metal Charge Transfer in Trinuclear Mixed-Valent Complexes. Inorganic Chemistry, 2023, 62, 4799-4813. | 1.9 | 2 |
| 17526 | Theoretical Spectroscopy Aided Validation of the Hydration Structure of Trimethylamine N° -Oxide (TMAO). Journal of Physical Chemistry B, 2023, 127, 2774-2783. | 1.2 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17527 | Decomposing Chemical Space: Applications to the Machine Learning of Atomic Energies. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 2029-2038. | 2.3 | 3 |
| 17528 | Amide and Urea Based Solvents for Li ⁺ O ²⁻ Batteries. Part II: Evaluation of Decomposition Pathways Using Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2023, 127, 7043-7053. | 1.5 | 2 |
| 17529 | The Origin of Anion ⁻ Autocatalysis. <i>Jacs Au</i> , 2023, 3, 1039-1051. | 3.6 | 5 |
| 17530 | Electrophilicity and nucleophilicity scales at different DFT computational levels. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, . | 0.9 | 12 |
| 17531 | ReDD-COFFEE: a ready-to-use database of covalent organic framework structures and accurate force fields to enable high-throughput screenings. <i>Journal of Materials Chemistry A</i> , 2023, 11, 7468-7487. | 5.2 | 7 |
| 17532 | Performance of Copper Corrosion Inhibitors on Pipecoridithiocarbamic Acid in 3 wt% NaCl Solution. <i>Electrochemistry</i> , 2023, , . | 0.6 | 0 |
| 17533 | Pd/Xu-Phos-catalyzed asymmetric elimination of fully substituted enol triflates into axially chiral trisubstituted allenes. <i>Science Advances</i> , 2023, 9, . | 4.7 | 6 |
| 17534 | Sulfonamide derived Schiff base Mn (II), Co (II), and Ni (II) complexes: Crystal structures, density functional theory and Hirshfeld surface analysis. <i>Applied Organometallic Chemistry</i> , 2023, 37, . | 1.7 | 13 |
| 17535 | Controllable Aggregation-Induced Emission and Förster Resonance Energy Transfer Behaviors of Bistable [2] Daisy Chain Rotaxanes for White-Light Emission and Temperature-Sensing Applications. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 15353-15366. | 4.0 | 5 |
| 17536 | Mechanistic Investigation into the Regio-Controllable Hydroallylations of Alkynes with Allylborons under Pd-Based Synergetic Catalyses. <i>Journal of Organic Chemistry</i> , 2023, 88, 4536-4545. | 1.7 | 1 |
| 17537 | Stereochemistry of the Reactions between Palladacycle Complexes and Primary Alkyl Iodides. <i>Organometallics</i> , 2023, 42, 606-614. | 1.1 | 0 |
| 17538 | Exciton States of Azobenzene Aggregates: A First-Principles Study. <i>Advanced Theory and Simulations</i> , 2023, 6, . | 1.3 | 2 |
| 17539 | Do Models beyond Hybrid Density Functionals Increase the Agreement with Experiment for Predicted NMR Chemical Shifts or Electric Field Gradient Tensors in Organic Solids?. <i>Journal of Physical Chemistry A</i> , 2023, 127, 2846-2858. | 1.1 | 8 |
| 17540 | Reducing Exact Two-Component Theory for NMR Couplings to a One-Component Approach: Efficiency and Accuracy. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 2010-2028. | 2.3 | 8 |
| 17541 | Tuning anticancer properties and DNA-binding of Pt(II) complexes via alteration of nitrogen softness/basicity of tridentate ligands. <i>RSC Advances</i> , 2023, 13, 9333-9346. | 1.7 | 2 |
| 17542 | Crystal Structure, DFT Investigation, Molecular Docking, Antioxidant and Thrombolytic Investigation of Thioxo Pyrimidine-5-Carboxylate. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-14. | 1.4 | 0 |
| 17543 | A DFT study of structural-stability, Mulliken charges, MEP, FMO, and NLO properties of trans alkenyl substituted chalcones conformers: theoretical study. <i>Structural Chemistry</i> , 0, , . | 1.0 | 1 |
| 17544 | Molecular Docking, DFT, and Antibacterial Activity Study of a Newly Synthesized Mixed Ligand Complex of Co(II), 1,10-Phenanthroline, Adenine and Acetamide. <i>Chemistry Africa</i> , 0, , . | 1.2 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 17545 | Multiple resonance induced thermally activated delayed fluorescence: effect of chemical modification. <i>Electronic Structure</i> , 2023, 5, 014010. | 1.0 | 1 |
| 17546 | Helical allophycocyanin nanotubes absorb far-red light in a thermophilic cyanobacterium. <i>Science Advances</i> , 2023, 9, . | 4.7 | 6 |
| 17547 | Modulation of metal species as control point for Ni-catalyzed stereodivergent semihydrogenation of alkynes with water. <i>Nature Communications</i> , 2023, 14, . | 5.8 | 11 |
| 17549 | Comprehensive exploration of graphically defined reaction spaces. <i>Scientific Data</i> , 2023, 10, . | 2.4 | 9 |
| 17550 | Interpreting vibrational circular dichroism spectra: the Cai factor for absolute configuration with confidence. <i>Journal of Cheminformatics</i> , 2023, 15, . | 2.8 | 0 |
| 17551 | Noncollinear and Spin-Flip TDDFT in Multicollinear Approach. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 2270-2281. | 2.3 | 2 |
| 17552 | Propane Oxidative Dehydrogenation on Nanosized Boron Carbide: Effect of Boron Content and Its Oxidation Implicated by DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2023, 127, 6280-6293. | 1.5 | 0 |
| 17553 | Diserinol Isophthalamide: A Novel Reagent for Complexation with Biomolecular Anions in Electrospray Ionization Mass Spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2023, 34, 745-753. | 1.2 | 0 |
| 17555 | Photoluminescence Properties of Single-Walled Carbon Nanotubes Influenced by the Tether Length of Reagents with Two Reactive Sites. <i>Chemistry - A European Journal</i> , 2023, 29, . | 1.7 | 4 |
| 17556 | A density functional theory insight into the extraction mechanism of lithium recovery from alkaline brine by β -diketones. <i>AIChE Journal</i> , 2023, 69, . | 1.8 | 2 |
| 17557 | Toward a Combined Molecular Dynamics and Quantum Mechanical Approach to Understanding Solvent Effects on Chemical Processes in the Pharmaceutical Industry: The Case of a Lewis Acid-Mediated S_NAr Reaction. <i>Organic Process Research and Development</i> , 2023, 27, 742-754. | 1.3 | 0 |
| 17558 | DNA Binding and Cleavage, Stopped-Flow Kinetic, Mechanistic, and Molecular Docking Studies of Cationic Ruthenium(II) Nitrosyl Complexes Containing ϵ -NS ₄ -Core. <i>Molecules</i> , 2023, 28, 3028. | 1.7 | 1 |
| 17559 | Defect engineering in MIL-125-(Ti)-NH ₂ for enhanced photocatalytic H ₂ generation. <i>Journal of Materials Chemistry A</i> , 2023, 11, 9143-9151. | 5.2 | 11 |
| 17560 | Cytotoxicity and Antibacterial Potentials of Mixed Ligand Cu(II) and Zn(II) Complexes: A Combined Experimental and Computational Study. <i>ACS Omega</i> , 2023, 8, 13421-13434. | 1.6 | 2 |
| 17561 | <i>meso</i> -Carbazole decorated BODIPYs as an electron donor-acceptor system with excellent fluorosolvato/vapochromic behavior, aggregation-induced emission, and antileishmanial activity. <i>New Journal of Chemistry</i> , 2023, 47, 8277-8290. | 1.4 | 2 |
| 17562 | A host-dye complex for sensitive fluorescence detection and clearing of spermine in cells. <i>Sensors and Actuators B: Chemical</i> , 2023, 386, 133757. | 4.0 | 7 |
| 17563 | Electroluminescence of Tetradentate Pt(II) Complexes: O ^N N ^O versus C ^N N ^O Coordination. <i>Inorganic Chemistry</i> , 2023, 62, 5772-5779. | 1.9 | 6 |
| 17564 | Amino acids assisted growth of methylammonium lead iodide cuboidal crystals for solar cell applications. <i>Chemical Physics</i> , 2023, 571, 111914. | 0.9 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 17565 | Unraveling the Molecular Mechanism of <i>S</i> -Nitrosation Mediated by <i>N</i> -Acetylmicroperoxidase-11. <i>Inorganic Chemistry</i> , 2023, 62, 5630-5643. | 1.9 | 1 |
| 17567 | A Metastable Ketenyl Radical-Water Complex from UV Photolysis of the Carboxymethyl Radical. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3171-3178. | 1.1 | 0 |
| 17568 | A post synthetically modified metal-organic framework as an efficient hydrogen evolution reaction catalyst in all pH conditions. <i>New Journal of Chemistry</i> , 0, , . | 1.4 | 0 |
| 17569 | Corrosion Inhibiting by Some Organic Heterocyclic Inhibitors Through Langmuir Adsorption Mechanism on the Al-X (X = Mg/Ga/Si) Alloy Surface: A Study of Quantum Three-Layer Method of CAM-DFT/ONIOM. <i>Journal of Bio- and Tribo-Corrosion</i> , 2023, 9, . | 1.2 | 8 |
| 17570 | Investigating the Thermodynamics and Kinetics of Catechin Pyrolysis for Environmentally Friendly Binders. <i>ACS Omega</i> , 2023, 8, 12693-12701. | 1.6 | 0 |
| 17571 | Thieno[2,3- <i>c</i>]isoquinolines: A novel chemotype of antiproliferative agents inducing cellular apoptosis while targeting the G2/M phase and Tubulin. <i>Drug Development Research</i> , 0, , . | 1.4 | 0 |
| 17572 | Nanocomposites with ZrO ₂ @S-Doped g-C ₃ N ₄ as an Enhanced Binder-Free Sensor: Synthesis and Characterization. <i>ACS Omega</i> , 2023, 8, 13775-13790. | 1.6 | 7 |
| 17574 | Synthesis of extended covalently bound porphyrins on Au(111) surface. <i>Materials Advances</i> , 0, , . | 2.6 | 0 |
| 17575 | Nematic phase of polar unsymmetrical bent-core molecules. <i>ChemPhysChem</i> , 0, , . | 1.0 | 1 |
| 17576 | Deciphering and investigating fragment mechanism of quinolones using multi-collision energy mass spectrometry and computational chemistry strategy. <i>Rapid Communications in Mass Spectrometry</i> , 2023, 37, . | 0.7 | 1 |
| 17577 | Twisted intramolecular charge-transfer state of <i>trans</i> - <i>N,N'</i> -bis(2-ethylphenyl)ethylenediamine. <i>Journal of Physical Chemistry A</i> , 2023, 127, 10000-10006. | 0.8 | 0 |
| 17578 | Influence of Core Topologies on Poly-l-lysine Dendrimer Structures. <i>Journal of Physical Chemistry B</i> , 2023, 127, 3364-3371. | 1.2 | 0 |
| 17579 | Synthesis and characterization of cobalt (II) pincer complexes and their application as dyes in dye-sensitized solar cells. <i>Journal of Molecular Structure</i> , 2023, 1286, 135508. | 1.8 | 4 |
| 17580 | Polarity and Dielectric Property Control Triggered by a Coordinated Solvent Molecule Exchange in Luminescent Mononuclear Aluminium(III) Complexes. <i>Chemistry - A European Journal</i> , 0, , . | 1.7 | 0 |
| 17581 | CuF ₂ /MeOH-Catalyzed N ³ -Selective Chan-Lam Coupling of Hydantoins: Method and Mechanistic Insight. <i>Journal of Organic Chemistry</i> , 2023, 88, 6058-6070. | 1.7 | 3 |
| 17582 | Efficient Band-Edge Emission from Indirect Bandgap Semiconductor Quantum Dots upon Shell Engineering. <i>Nano Letters</i> , 2023, 23, 3239-3244. | 4.5 | 3 |
| 17583 | Polyethylene Glycol 20k. Does It Fluoresce?. <i>ACS Omega</i> , 2023, 8, 14208-14218. | 1.6 | 1 |
| 17584 | The relationships between direct substituents, aromaticity and kinetic stability of pentazole ring. <i>FirePhysChem</i> , 2023, 3, 350-355. | 1.5 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17585 | DFT Study on the Mechanisms of Iron-Catalyzed Ortho C-H Homoallylation of Aromatic Ketones with Methylenecyclopropanes. <i>Organometallics</i> , 2023, 42, 632-640. | 1.1 | 1 |
| 17586 | Selective Heating Effect of Microwave Irradiation on Binary Mixture of Water and Polyethylene Oxide: Molecular Dynamics Simulation Approach. <i>Physical Chemistry Chemical Physics</i> , 0, , . | 1.3 | 0 |
| 17587 | A customized MOF-polymer composite for rapid gold extraction from water matrices. <i>Science Advances</i> , 2023, 9, . | 4.7 | 18 |
| 17588 | Molecular Engineering to Tune Functionality: The Case of Cl-Substituted [Fe(terpy) ₂] ²⁺ . <i>Inorganic Chemistry</i> , 2023, 62, 6397-6410. | 1.9 | 3 |
| 17589 | Mechanism of pH influence on aptamer binding with Cd ²⁺ revealed by molecular dynamics simulation. <i>New Journal of Chemistry</i> , 2023, 47, 9239-9249. | 1.4 | 2 |
| 17590 | Magnetic Polaron States in Photoluminescent Carbon Dots Enable Hydrogen Peroxide Photoproduction. <i>Small</i> , 2023, 19, . | 5.2 | 2 |
| 17591 | Organic-inorganic hybrid salt and mixed ligand Cr(III) complexes containing the natural flavonoid chrysin: Synthesis, characterization, computational, and biological studies. <i>Frontiers in Chemistry</i> , 0, 11, . | 1.8 | 1 |
| 17592 | Spectral Characteristics and Functional Responses of Phospholipid Bilayers in the Terahertz Band. <i>International Journal of Molecular Sciences</i> , 2023, 24, 7111. | 1.8 | 0 |
| 17593 | Evidence of a Wheland Intermediate in Carboxylate-Assisted C(sp ²)-H Activation by Pd(IV) Active Catalyst Species Studied via DFT Calculations. <i>Catalysts</i> , 2023, 13, 724. | 1.6 | 0 |
| 17594 | Synthesis of natural glucomannan derivative as a highly-efficient green inhibitor for mild steel in the simulated seawater. <i>Journal of Industrial and Engineering Chemistry</i> , 2023, 124, 132-146. | 2.9 | 2 |
| 17595 | Removal of oxygen-containing functional groups during hydrothermal carbonization of biomass: Experimental and DFT study. <i>Energy</i> , 2023, 276, 127436. | 4.5 | 4 |
| 17596 | Dynamical Simulations of Carotenoid Photoexcited States Using Density Matrix Renormalization Group Techniques. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3714-3727. | 1.1 | 3 |
| 17597 | Design and synthesis of photostable triphenylamine based neutral AIE nano luminogens: specific and long-term tracking of mitochondria in cells. <i>Biomaterials Science</i> , 2023, 11, 3938-3951. | 2.6 | 3 |
| 17599 | Reduction of Bacterial Folic Acid Production and Cell Membrane Disruption of <i>Klebsiella pneumoniae</i> by Two Amino Substituted Pyridyl Compounds: An Experimental and In Silico Approach. <i>Chemistry Africa</i> , 2023, 6, 2725-2735. | 1.2 | 3 |
| 17600 | Experimental and Theoretical Study on Crown Ether-Appended-Fe(III) Porphyrin Complexes and Catalytic Oxidation Cyclohexene with O ₂ . <i>Molecules</i> , 2023, 28, 3452. | 1.7 | 0 |
| 17601 | Real-Time Time-Dependent Density Functional Theories With Large Time Step and Short Simulation Time. , 2024, , 229-257. | | 0 |
| 17602 | Spectroscopical and Molecular Studies of Four Manganese(I) PhotoCORMs with Bioinspired Ligands Containing Non-Coordinated Phenol Groups. <i>Molecules</i> , 2023, 28, 3439. | 1.7 | 0 |
| 17603 | Mechanism of metalated pyrrole-singlet oxygen chemiluminescent reaction. <i>Polyhedron</i> , 2023, 238, 116421. | 1.0 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|-----|-----------|
| 17604 | A novel calculation strategy for optimized prediction of the reduction of electrochemical window at anode. Chinese Physics B, 0, , . | 0.7 | 1 |
| 17605 | Virtual screening of organic quinones as cathode materials for sodium-ion batteries. Energy Advances, 2023, 2, 820-828. | 1.4 | 3 |
| 17606 | Clay-supported acidic ionic liquid as an efficient catalyst for conversion of carbohydrates to 5-hydroxymethylfurfural. Journal of Molecular Liquids, 2023, 382, 121847. | 2.3 | 14 |
| 17607 | Enantiodivergent Photochemical Rearrangements Due to Different Coordination Modes at an Oxazaborolidine Lewis Acid Catalyst. ACS Catalysis, 0, , 5896-5905. | 5.5 | 0 |
| 17608 | DFT insight of hydroxide degradation pathways for heterocyclic quaternary ammonium cations in anion exchange membranes. Journal of Membrane Science, 2023, 678, 121672. | 4.1 | 6 |
| 17609 | Prediction of CO ₂ with amine functionalized ionic liquids interaction using density functional theory. Case Studies in Chemical and Environmental Engineering, 2023, 8, 100355. | 2.9 | 2 |
| 17610 | A DFT study on the reaction mechanism of the gold(I)-catalyzed cycloisomerization of alkynylhydroxyallylamides to 4-oxa-6-azatricyclo[3.3.0.0 ^{2,8}]octane and 3-acyl-4-alkenylpyrrolidine. Journal of the Chinese Chemical Society, 2023, 70, 1558-1567. | 0.8 | 0 |
| 17611 | Thermochemistry of the Smallest Hyperbolic Paraboloid Hydrocarbon: A High-Level Quantum Chemical Perspective. Journal of Carbon Research, 2023, 9, 41. | 1.4 | 0 |
| 17612 | Constrained density functional theory calculations for estimation of forward and backward intermolecular charge transfer energy. Bulletin of the Korean Chemical Society, 0, , . | 1.0 | 0 |
| 17613 | Emergent solvation phenomena in non-aqueous electrolytes with multiple anions. CheM, 2023, 9, 1955-1971. | 5.8 | 7 |
| 17614 | Computational Study on a Transfer Hydrogenation Catalysed by a Ru(II) Bis-Pyrazolyl Pyridine Complex. Israel Journal of Chemistry, 0, , . | 1.0 | 0 |
| 17615 | Spectroscopic (FT-IR, FT-Raman, UV-vis and NMR) Investigation, Molecular Structure, Docking and Chemical Reactivity Elucidation of Antifungal Drug Tioconazole. Polycyclic Aromatic Compounds, 0, , 1-25. | 1.4 | 0 |
| 17616 | Synthesis and Characterization of a Rhenanaphthalene Isomer. Chemistry - A European Journal, 2023, 29, . | 1.7 | 0 |
| 17617 | Photofragmentation specificity of photoionized cyclic amino acids (diketopiperazines) as precursors of peptide building blocks. Physical Chemistry Chemical Physics, 2023, 25, 15635-15646. | 1.3 | 1 |
| 17618 | A multi responsive phosphonic acid based fluorescent sensor for sensing Fe ³⁺ , benzaldehyde and antibiotics. Microchemical Journal, 2023, 191, 108771. | 2.3 | 4 |
| 17619 | Substituent effects in the tautomerization of imidic acids R ² C(OH)=NH ↔ R ² C(O)NH ₂ : Kinetic implications for the formation of peptide bonds in the interstellar medium. International Journal of Chemical Kinetics, 2023, 55, 381-391. | 1.0 | 4 |
| 17620 | An experimental and theoretical investigation of the N(² D) + C ₆ H ₆ (benzene) reaction with implications for the photochemical models of Titan. Faraday Discussions, 0, 245, 327-351. | 1.6 | 4 |
| 17621 | Meta-GGA Density Functional Calculations on Atoms with Spherically Symmetric Densities in the Finite Element Formalism. Journal of Chemical Theory and Computation, 2023, 19, 2502-2517. | 2.3 | 10 |

| # | ARTICLE | IF | CITATIONS |
|-------|---|-----|-----------|
| 17622 | Hydrogen-bonding receptor substituted BODIPYs as selective ON-OFF fluorimetric sensors for fluoride ions in polar aprotic organic solvents â€“ A molecular-level understanding based on experimental and theoretical studies. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 442, 114780. | 2.0 | 1 |
| 17623 | An efficient biochar adsorbent for CO ₂ capture: Combined experimental and theoretical study on the promotion mechanism of N-doping. <i>Chemical Engineering Journal</i> , 2023, 466, 143095. | 6.6 | 2 |
| 17681 | The Fully Oxidized State of the Glutamate Coordinated O ₂ -Tolerant [NiFe]-Hydrogenase Shows a Ni(III)/Fe(III) Open-Shell Singlet Ground State. <i>Journal of the American Chemical Society</i> , 2023, 145, 10954-10959. | 6.6 | 3 |
| 17682 | Pushing the boundaries of VCD spectroscopy in natural product chemistry. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 13825-13832. | 1.3 | 2 |
| 17701 | Predicting reactivity with a general-purpose reactivity indicator. , 2023, , 159-180. | | 1 |
| 17746 | Benchmarking Modern Density Functionals for Broad Applications in Chemistry. , 2024, , 78-93. | | 0 |
| 17765 | The effect of the presence of BF ₄ ⁻ and Cl ⁻ anions on the value of the thermodynamic functions of the 1,2,4-h-triazole Fe(II) complex. <i>AIP Conference Proceedings</i> , 2023, , . | 0.3 | 0 |
| 17768 | Hirshfeld atom refinement of metal-organic frameworks for accurate positioning of hydrogen atoms and disorder analysis. <i>Chemical Communications</i> , 2023, 59, 8799-8802. | 2.2 | 0 |
| 17772 | Approaching Coupled Cluster Accuracy with Density Functional Theory Using the Generalized Connectivity-Based Hierarchy. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 3763-3778. | 2.3 | 2 |
| 17854 | Electronic Structure-Antioxidant Action Relationships for Chemical Compounds. <i>Advances in Chemical and Materials Engineering Book Series</i> , 2023, , 143-158. | 0.2 | 0 |
| 17876 | A Computational Study of the Reaction Between N(2D) and Simple Aromatic Hydrocarbons. <i>Lecture Notes in Computer Science</i> , 2023, , 718-734. | 1.0 | 0 |
| 17878 | Computational Investigation of the $N_2 + C_2H_4$ and $N_2 + CH_2CHCN$ Reactions: Benchmark Analysis and Implications for Titan's Atmosphere. <i>Lecture Notes in Computer Science</i> , 2023, , 705-717. | 1.0 | 0 |
| 17940 | Review of Approximations for the Exchange-Correlation Energy in Density-Functional Theory. , 2023, , 1-90. | | 3 |
| 17969 | Binding energies for successive addition reactions of C_6OH to C ₆₀ : A laboratory for testing frontier molecular orbital theory. <i>Advances in Quantum Chemistry</i> , 2023, , . | 0.4 | 0 |
| 17998 | Chemoselectivity Streamlines the Approach to Linear and Y-Shaped Thiol-Polyethers Starting from Thiocarboxylic Acids. <i>ACS Macro Letters</i> , 0, , 1185-1192. | 2.3 | 1 |
| 18044 | Generalized Energy-Based Fragmentation Approach for Structures and Properties of Periodic Condensed Phase Systems. , 2024, , 129-138. | | 0 |
| 18046 | Modelling Methods for Flow Batteries. <i>Engineering Applications of Computational Methods</i> , 2023, , 65-126. | 0.5 | 0 |
| 18049 | Structural design of organic battery electrode materials: from DFT to artificial intelligence. <i>Rare Metals</i> , 2023, 42, 3269-3303. | 3.6 | 1 |

| # | ARTICLE | IF | CITATIONS |
|-------|--|------|-----------|
| 18193 | Relativistic Real-Time Methods. , 2024, , 200-228. | | 0 |
| 18245 | Development of Exchange-Correlation Functionals Assisted by Machine Learning. Challenges and Advances in Computational Chemistry and Physics, 2023, , 91-112. | 0.6 | 1 |
| 18422 | Investigation of the Conductive Properties of the Electro-Polymerized Thiophene and Pyrrole Derivatives: Correlation Between Experimental and Theoretical Parameters. Communications in Computer and Information Science, 2023, , 376-387. | 0.4 | 0 |
| 18435 | Ab Initio Calculations of Band Structures of Bulk BaTiO ₃ Based on Density Functional Theory with Hybrid Functional. , 2023, , . | | 0 |
| 18522 | Comonomer effects in vinyl based photocatalytic polymers. , 0, , . | | 0 |
| 18644 | Tetryliumylidene ions in synthesis and catalysis. Chemical Science, 2024, 15, 4275-4291. | 3.7 | 0 |
| 18683 | Computational chemistry for water-splitting electrocatalysis. Chemical Society Reviews, 2024, 53, 2771-2807. | 18.7 | 1 |
| 18698 | Density functional theory methods applied to homogeneous and heterogeneous catalysis: a short review and a practical user guide. Physical Chemistry Chemical Physics, 2024, 26, 7950-7970. | 1.3 | 0 |
| 18707 | Temperature-dependent hole mobility in pyrene- π -thiophene-based room-temperature discotic liquid crystals. Chemical Communications, 2024, 60, 2922-2925. | 2.2 | 0 |
| 18848 | Lightening calculations for Schiff base lanthanide complexes. AIP Conference Proceedings, 2024, , . | 0.3 | 0 |