# Double-hybrid density functionals with long-range disp accuracy and extended applicability

Physical Chemistry Chemical Physics

9, 3397

DOI: 10.1039/b704725h

Citation Report

| # | Article | IF | Citations |
|---|---|---|---|
| 12 | Double-hybrid density functional theory for excited electronic states of molecules. Journal of Chemical Physics, 2007, 127, 154116. | 1.2 | 404 |
| 13 | A unified density-functional treatment of dynamical, nondynamical, and dispersion correlations. Journal of Chemical Physics, 2007, 127, 124108. | 1.2 | 193 |
| 14 | Structure and binding energies of the porphine dimer. Molecular Physics, 2007, 105, 2793-2798. | 0.8 | 31 |
| 15 | A Theoretical Study on the Electronic Structure of Auâ˜XO(0,-1,+1)Â(X = C, N, and O) Complexes:Â Effect of an External Electric Field. Journal of Physical Chemistry A, 2007, 111, 13255-13263. | 1.1 | 27 |
| 16 | How strong is the bond between water and salt?. Surface Science, 2008, 602, L135-L138. | 0.8 | 21 |
| 17 | Metal induced molecular nano-extraction. Theoretical Chemistry Accounts, 2008, 121, 247-255. | 0.5 | 1 |
| 18 | Ab initio analysis of the Cope rearrangement of germacrane sesquiterpenoids. Journal of Molecular Modeling, 2008, 14, 335-342. | 0.8 | 30 |
| 19 | Latest developments and applications of double-hybrid density functionals. Chemistry Central Journal, 2008, 2, . | 2.6 | 0 |
| 20 | Natural orbital functional description of van der Waals interactions: A case study of the effect of the basis set for the helium dimer. International Journal of Quantum Chemistry, 2008, 108, 1660-1663. | 1.0 | 14 |
| 21 | Calculation of conformational energies and optical rotation of the most simple chiral alkane. Chirality, 2008, 20, 1009-1015. | 1.3 | 33 |
| 22 | Theoretical Description of Substituent Effects in Electrophilic Aromatic Substitution Reactions. European Journal of Organic Chemistry, 2008, 2008, 5928-5935. | 1.2 | 10 |
| 23 | Do Special Noncovalent Ï€â€“Ï€ Stacking Interactions Really Exist?. Angewandte Chemie - International Edition, 2008, 47, 3430-3434. | 7.2 | 928 |
| 24 | Chirality Recognition between Neutral Molecules in the Gas Phase. Angewandte Chemie - International Edition, 2008, 47, 6970-6992. | 7.2 | 221 |
| 27 | Long-range corrected hybrid density functionals with damped atomâ€“atom dispersion corrections. Physical Chemistry Chemical Physics, 2008, 10, 6615. | 1.3 | 10,464 |
| 28 | Performance of B3LYP Density Functional Methods for a Large Set of Organic Molecules. Journal of Chemical Theory and Computation, 2008, 4, 297-306. | 2.3 | 931 |
| 29 | Implementation and Performance of DFT-D with Respect to Basis Set and Functional for Study of Dispersion Interactions in Nanoscale Aromatic Hydrocarbons. Journal of Chemical Theory and Computation, 2008, 4, 2030-2048. | 2.3 | 161 |
| 30 | 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. Journal of Physical Chemistry A, 2008, 112, 12868-12886. | 1.1 | 680 |
| 31 | Searching of potential energy curves for the benzene dimer using dispersion-corrected density functional theory. Physical Chemistry Chemical Physics, 2008, 10, 2715. | 1.3 | 25 |

| # | Article | IF | Citations |
|---|---|---|---|
| 32 | Calculating stacking interactions in nucleic acid base-pair steps using spin-component scaling and local second order MÃ¸llerâ€“Plesset perturbation theory. Physical Chemistry Chemical Physics, 2008, 10, 2785. | 1.3 | 45 |
| 33 | B3LYP augmented with an empirical dispersion term (B3LYP-D*) as applied to molecular crystals. CrystEngComm, 2008, 10, 405-410. | 1.3 | 775 |
| 34 | Structures and interaction energies of stacked grapheneâ€“nucleobase complexes. Physical Chemistry Chemical Physics, 2008, 10, 2722. | 1.3 | 258 |
| 35 | Assessment of Density Functionals for Intramolecular Dispersion-Rich Interactions. Journal of Chemical Theory and Computation, 2008, 4, 1610-1619. | 2.3 | 65 |
| 36 | Empirical Corrections to Density Functional Theory Highlight the Importance of Nonbonded Intramolecular Interactions in Alkanes. Journal of Physical Chemistry A, 2008, 112, 11495-11500. | 1.1 | 48 |
| 37 | Toward the Exact Solution of the Electronic SchrÃ¶dinger Equation for Noncovalent Molecular Interactions:â€‰ Worldwide Distributed Quantum Monte Carlo Calculations. Journal of Physical Chemistry A, 2008, 112, 2104-2109. | 1.1 | 47 |
| 38 | Analysis of non-covalent interactions in (bio)organic molecules using orbital-partitioned localized MP2. Physical Chemistry Chemical Physics, 2008, 10, 3327. | 1.3 | 51 |
| 39 | Interactions in Large, Polyaromatic Hydrocarbon Dimers: Application of Density Functional Theory with Dispersion Corrections. Journal of Physical Chemistry A, 2008, 112, 10968-10976. | 1.1 | 136 |
| 40 | Elementary Peptide Motifs in the Gas Phase: FTIR Aggregation Study of Formamide, Acetamide, N-Methylformamide, and N-Methylacetamide. Journal of Physical Chemistry A, 2008, 112, 7530-7542. | 1.1 | 79 |
| 41 | Exploring the Limit of Accuracy of the Global Hybrid Meta Density Functional for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2008, 4, 1849-1868. | 2.3 | 956 |
| 42 | Intermolecular Potentials. Science, 2008, 321, 787-789. | 6.0 | 119 |
| 43 | Quantum chemical studies on hydrogen adsorption in carbon-based model systems: role of charged surface and the electronic induction effect. Physical Chemistry Chemical Physics, 2008, 10, 5832. | 1.3 | 44 |
| 44 | Dispersion energy from density-fitted density susceptibilities of singles and doubles coupled cluster theory. Journal of Chemical Physics, 2008, 128, 144107. | 1.2 | 61 |
| 45 | IR/UV spectra and quantum chemical calculations of Trpâ€“Ser: Stacking interactions between backbone and indole side-chain. Physical Chemistry Chemical Physics, 2008, 10, 2844. | 1.3 | 35 |
| 46 | Influence of Sequential Guanidinium Methylation on the Energetics of the GuanidiniumÂ·Â·Â·Guanine Dimer and GuanidiniumÂ·Â·Â·GuanineÂ·Â·Â·Cytosine Trimer: Implications for the Control of ProteinÂ·Â·Â·DNA Interactions by Arginine Methyltransferases. Journal of Physical Chemistry B, 2008, 112, 16995-17002. | 1.2 | 3 |
| 47 | Raman spectral evidence of methyl rotation in liquid toluene. Physical Chemistry Chemical Physics, 2008, 10, 1003-1008. | 1.3 | 26 |
| 48 | Tighter multipole-based integral estimates and parallel implementation of linear-scaling AOâ€“MP2 theory. Physical Chemistry Chemical Physics, 2008, 10, 3335. | 1.3 | 74 |
| 49 | Stereochemical Nonrigidity of a Chiral Rhodium Boryl Hydride Complex:Â AÏƒ-Borane Complex as Transition State for Isomerization. Journal of the American Chemical Society, 2008, 130, 4375-4385. | 6.6 | 20 |

| # | Article | IF | Citations |
|---|---|---|---|
| 50 | Physisorption and Chemisorption of Hydrocarbons in H-FAU Using QM-Pot(MP2//B3LYP) Calculations. Journal of Physical Chemistry C, 2008, 112, 11796-11812. | 1.5 | 55 |
| 51 | On the Importance of Electron Correlation Effects for the Intramolecular Stacking Geometry of a Bis-Thiophene Derivative. Journal of Physical Chemistry A, 2008, 112, 12469-12474. | 1.1 | 23 |
| 52 | Semiempirical Double-Hybrid Density Functional with Improved Description of Long-Range Correlation. Journal of Physical Chemistry A, 2008, 112, 2702-2712. | 1.1 | 123 |
| 53 | Theoretical Thermodynamics for Large Molecules: Walking the Thin Line between Accuracy and Computational Cost. Accounts of Chemical Research, 2008, 41, 569-579. | 7.6 | 329 |
| 54 | Bond Dissociation Enthalpies of Large Aromatic Carbon-Centered Radicals. Journal of Physical Chemistry A, 2008, 112, 13566-13573. | 1.1 | 35 |
| 56 | Van der Waals Interactions in DFT Made Easy by Wannier Functions. Physical Review Letters, 2008, 100, 053002. | 2.9 | 189 |
| 57 | Quantum Chemical Benchmark Energy and Geometry Database for Molecular Clusters and Complex Molecular Systems (www.begdb.com): A Users Manual and Examples. Collection of Czechoslovak Chemical Communications, 2008, 73, 1261-1270. | 1.0 | 144 |
| 59 | Assessment of double-hybrid energy functionals for Ï€-conjugated systems. Journal of Chemical Physics, 2009, 131, 084108. | 1.2 | 74 |
| 60 | On the self-consistent implementation of general occupied-orbital dependent exchange-correlation functionals with application to the B05 functional. Journal of Chemical Physics, 2009, 131, 084103. | 1.2 | 25 |
| 61 | Long-range-corrected hybrid density functionals including random phase approximation correlation: Application to noncovalent interactions. Journal of Chemical Physics, 2009, 131, 034110. | 1.2 | 82 |
| 62 | Doubly hybrid density functional for accurate descriptions of nonbond interactions, thermochemistry, and thermochemical kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 4963-4968. | 3.3 | 332 |
| 63 | The structure of phenol-Arnâ€ˆ(n=1,2) clusters in their S and S1 states. Journal of Chemical Physics, 2009, 130, 224303. | 1.2 | 38 |
| 64 | Development and assessment of a short-range meta-GGA functional. Journal of Chemical Physics, 2009, 130, 234112. | 1.2 | 48 |
| 65 | Further analysis and comparative study of intermolecular interactions using dimers from the S22 database. Journal of Chemical Physics, 2009, 131, 065102. | 1.2 | 82 |
| 66 | Assignment of the absolute configuration of zwitterionic and neutral macropodumines by means of TDDFT CD calculations. Chirality, 2009, 21, 561-568. | 1.3 | 20 |
| 67 | On the Importance of Ribose Orientation in the Substrate Activation of the Coenzyme B<sub>12</sub>â€Dependent Mutases. Chemistry - A European Journal, 2009, 15, 8578-8585. | 1.7 | 23 |
| 68 | Computational Investigation of Hydrogen Adsorption by Alkaliâ€Metalâ€Doped Organic Molecules: Role of Aromaticity. ChemPhysChem, 2009, 10, 427-435. | 1.0 | 38 |
| 69 | A new hybrid DFT approach to electronic excitation and first hyperpolarizabilities of transition metal complexes. Journal of Computational Chemistry, 2009, 30, 2056-2063. | 1.5 | 27 |

| # | Article | IF | Citations |
|---|---|---|---|
| 70 | Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for zinc complexes. Journal of Computational Chemistry, 2009, 30, 2752-2763. | 1.5 | 51 |
| 71 | A perspective on the link between the exchange(-correlation) hole and dispersion forces. Journal of Mathematical Chemistry, 2009, 46, 86-96. | 0.7 | 20 |
| 72 | Dispersion interactions in densityâ€functional theory. Journal of Physical Organic Chemistry, 2009, 22, 1127-1135. | 0.9 | 322 |
| 73 | Modeling of a TrÃ¶gerâ€™s tweezer and its complexation properties. Journal of Molecular Structure, 2009, 934, 117-122. | 1.8 | 16 |
| 74 | Model study on sorption of polycyclic aromatic hydrocarbons to goethite. Journal of Colloid and Interface Science, 2009, 330, 244-249. | 5.0 | 37 |
| 75 | Ifrac"uv double resonance spectra of pyrazine dimers: Competition between <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si13.gif" display="inline" overflow="scroll"><mml:mrow><mml:mtext>CH</mml:mtext><mml:mo>â¯</mml:mo><mml:mi mathvariant="normal">Ï€</mml:mi></mml:mrow></mml:math>, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si14.gif" display="inline" overflow="scroll"><mml:mrow><mml:mi | 1.2 | 16 |
| 76 | Toward spectroscopic studies of biologically relevant systems: Vibrational spectrum of adenine as a test case for performances of long-range/dispersion corrected density functionals. Chemical Physics Letters, 2009, 475, 105-110. | 1.2 | 48 |
| 77 | â€œMindlessâ€•DFT Benchmarking. Journal of Chemical Theory and Computation, 2009, 5, 993-1003. | 2.3 | 215 |
| 78 | Conformational properties of six-membered heterocycles: accurate relative energy differences with DFT, the importance of dispersion interactions and silicon substitution effects. Physical Chemistry Chemical Physics, 2009, 11, 8689. | 1.3 | 60 |
| 79 | Conformational Isomerization of 5-Phenyl-1-pentene Probed by SEP-Population Transfer Spectroscopy. Journal of Physical Chemistry A, 2009, 113, 126-134. | 1.1 | 5 |
| 80 | Atomic-Scale Modeling of the Interaction between Short Polypeptides and Carbon Surfaces. Journal of Physical Chemistry B, 2009, 113, 12105-12112. | 1.2 | 34 |
| 81 | Quantum Chemical Study of Trimolecular Reaction Mechanism between Nitric Oxide and Oxygen in the Gas Phase. Journal of Physical Chemistry A, 2009, 113, 9092-9101. | 1.1 | 42 |
| 82 | Ion-Pair Binding Energies of Ionic Liquids: Can DFT Compete with Ab Initio-Based Methods?. Journal of Physical Chemistry A, 2009, 113, 7064-7072. | 1.1 | 163 |
| 83 | The Remarkable Cis Effect in the Ene Reactions of Nitrosocarbonyl Intermediates. Journal of Organic Chemistry, 2009, 74, 2301-2310. | 1.7 | 20 |
| 84 | Performance of Ab Initio and Density Functional Methods for Conformational Equilibria of C<sub>n</sub>H<sub>2n+2</sub> Alkane Isomers (n = 4â^’8). Journal of Physical Chemistry A, 2009, 113, 11974-11983. | 1.1 | 156 |
| 85 | Local Hybrid Functionals with an Explicit Dependence on Spin Polarization. Journal of Physical Chemistry A, 2009, 113, 11898-11906. | 1.1 | 43 |
| 86 | Origin of the Argon Nanocoating Shift in the OH Stretching Fundamental of n-Propanol: A Combined Experimental and Quantum Chemical Study. Journal of Physical Chemistry C, 2009, 113, 10929-10938. | 1.5 | 23 |
| 87 | Accurate Calculations of Intermolecular Interaction Energies Using Explicitly Correlated Coupled Cluster Wave Functions and a Dispersion-Weighted MP2 Method. Journal of Physical Chemistry A, 2009, 113, 11580-11585. | 1.1 | 150 |

| # | Article | IF | Citations |
|---|---|---|---|
| 88 | Understanding the Role of Intra- and Intermolecular Interactions in the Formation of Single- and Double-Helical Structures of Aromatic Oligoamides: A Computational Study. Journal of Physical Chemistry A, 2009, 113, 1335-1342. | 1.1 | 24 |
| 89 | Accurate Quantum Chemical Description of Non-Covalent Interactions in Hydrogen Filled Endohedral Fullerene Complexes. Journal of Physical Chemistry C, 2009, 113, 17006-17010. | 1.5 | 63 |
| 90 | H/Br Exchange in BBr<sub>3</sub> by HSiR<sub>3</sub> (R = H, CH<sub>3</sub>,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 667 Td (C<s Barrier. Journal of Physical Chemistry A, 2009, 113, 12035-12043. | 1.1 | 12 |
| 91 | Unified Inter- and Intramolecular Dispersion Correction Formula for Generalized Gradient Approximation Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 2950-2958. | 2.3 | 76 |
| 92 | Benzeniumâˆ'Ethene Complex: A Fundamental Problem for Standard Second-Order MÃ¸llerâˆ'Plesset Theory. Journal of Physical Chemistry A, 2009, 113, 3005-3008. | 1.1 | 19 |
| 93 | Coulomb-only second-order perturbation theory in long-range-corrected hybrid density functionals. Physical Chemistry Chemical Physics, 2009, 11, 9677. | 1.3 | 29 |
| 94 | Implementation and Optimization of DFT-D/COSab with Respect to Basis Set and Functional: Application to Polar Processes of Furfural Derivatives in Solution. Journal of Chemical Theory and Computation, 2009, 5, 2772-2786. | 2.3 | 9 |
| 95 | Long-range corrected double-hybrid density functionals. Journal of Chemical Physics, 2009, 131, 174105. | 1.2 | 327 |
| 96 | Metallo[endo]fullereneâˆ'Amino Acid Interactions. A Theoretical Study. Journal of Physical Chemistry C, 2009, 113, 504-511. | 1.5 | 7 |
| 97 | van der Waals Interactions in Density Functional Theory Using Wannier Functions. Journal of Physical Chemistry A, 2009, 113, 5224-5234. | 1.1 | 80 |
| 98 | Examination of DFT and TDDFT Methods II. Journal of Physical Chemistry A, 2009, 113, 10873-10879. | 1.1 | 19 |
| 99 | 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 |
| 100 | Autocatalytic degradation of white phosphorus with silylenes. Physical Chemistry Chemical Physics, 2009, 11, 5273. | 1.3 | 25 |
| 101 | Benchmark Thermochemistry of the C<sub>n</sub>H<sub>2n+2</sub> Alkane Isomers (n = 2â˜'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 |
| 102 | Non covalent interactions in RNA and DNA base pairs: a quantum-mechanical study of the coupling between solvent and electronic density. Physical Chemistry Chemical Physics, 2009, 11, 11617. | 1.3 | 27 |
| 103 | Non-Covalent Interactions with Dual-Basis Methods: Pairings for Augmented Basis Sets. Journal of Chemical Theory and Computation, 2009, 5, 1560-1572. | 2.3 | 39 |
| 104 | The Structure of the Protonated Adenine Dimer by Infrared Multiple Photon Dissociation Spectroscopy and Electronic Structure Calculations. Journal of Physical Chemistry A, 2009, 113, 8099-8107. | 1.1 | 34 |
| 105 | A DFT study on the mechanism of a novel, regioselective, intramolecular Nâ€“Î€ rearrangement of cis and trans-Î·1-N-Cp*Rh-hydroxytamoxifen complexes to their Î·6 derivatives; potential breast cancer pharmaceuticals, and fluorescent probes. Dalton Transactions, 2009, , 4334. | 1.6 | 8 |

| # | Article | IF | Citations |
|---|---|---|---|
| 106 | Metalâ€“ligand cooperation in the trans addition of dihydrogen to a pincer Ir(i) complex: a DFT study. Dalton Transactions, 2009, , 9433. | 1.6 | 111 |
| 107 | Charge-transport properties of prototype molecular materials for organic electronics based on graphene nanoribbons. Physical Chemistry Chemical Physics, 2009, 11, 2741. | 1.3 | 47 |
| 108 | Role of dispersive interactions in layered materials: a periodic B3LYP and B3LYP-D* study of Mg(OH)2, Ca(OH)2 and kaolinite. Journal of Materials Chemistry, 2009, 19, 2564. | 6.7 | 75 |
| 109 | Hydrogen Bonding and Ï€-Stacking: How Reliable are Force Fields? A Critical Evaluation of Force Field Descriptions of Nonbonded Interactions. Journal of Chemical Information and Modeling, 2009, 49, 944-955. | 2.5 | 161 |
| 110 | Suitability of Double Hybrid Density Functionals and Their Dispersion-Corrected Counterparts in Producing the Potential Energy Curves for CO2â^'Rg (Rg: He, Ne, Ar and Kr) Systems. Journal of Physical Chemistry A, 2009, 113, 1377-1383. | 1.1 | 14 |
| 111 | Thiourea and isothiocyanate â€“ two useful chromophores for stereochemical studies. A comparison of experiment and computation. Organic and Biomolecular Chemistry, 2009, 7, 1562. | 1.5 | 15 |
| 112 | Recent developments of the quantum chemical cluster approach for modeling enzyme reactions. Journal of Biological Inorganic Chemistry, 2009, 14, 643-651. | 1.1 | 257 |
| 113 | Reaction Enthalpies Using the Neural-Network-Based X1 Approach: The Important Choice of Input Descriptors. Journal of Physical Chemistry A, 2009, 113, 3285-3290. | 1.1 | 19 |
| 114 | Good vibrations: probing biomolecular structure and interactions through spectroscopy in the gas phase. Molecular Physics, 2009, 107, 2435-2458. | 0.8 | 84 |
| 115 | Enantioselective HF Loss Promoted by Resonant Two-Photon Ionization of Supersonically Expanded (R)-1-Phenyl-2,2,2-trifluoroethanol Clusters. Journal of Physical Chemistry A, 2009, 113, 15127-15135. | 1.1 | 4 |
| 116 | TAMkin: A Versatile Package for Vibrational Analysis and Chemical Kinetics. Journal of Chemical Information and Modeling, 2010, 50, 1736-1750. | 2.5 | 155 |
| 117 | Palladium-Catalyzed Câ^'H Activation/Câ^'N Bond Formation Reactions: DFT Study of Reaction Mechanisms and Reactive Intermediates. Organometallics, 2010, 29, 821-834. | 1.1 | 67 |
| 118 | A Transferable H-Bonding Correction for Semiempirical Quantum-Chemical Methods. Journal of Chemical Theory and Computation, 2010, 6, 344-352. | 2.3 | 249 |
| 119 | A consistent and accurateab initioparametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. Journal of Chemical Physics, 2010, 132, 154104. | 1.2 | 35,972 |
| 120 | Conformational Properties of 1-Silyl-1-Silacyclohexane, C<sub>5</sub>H<sub>10</sub>SiHSiH<sub>3</sub>: Gas Electron Diffraction, Low-Temperature NMR, Temperature-Dependent Raman Spectroscopy, and Quantum Chemical Calculations. Journal of Physical Chemistry A, 2010, 114, 2127-2135. | 1.1 | 39 |
| 121 | Theoretical study of challenging properties of intramolecularly Ï€-stacked oligo(dibenzofulvene) organic molecular semiconductors. Theoretical Chemistry Accounts, 2010, 127, 605-612. | 0.5 | 7 |
| 122 | Overcoming systematic DFT errors for hydrocarbon reaction energies. Theoretical Chemistry Accounts, 2010, 127, 429-442. | 0.5 | 51 |
| 123 | Comparative semiempirical, ab initio, and density functional theory study on the thermodynamic properties of linear and branched perfluoroalkyl sulfonic acids/sulfonyl fluorides, perfluoroalkyl carboxylic acid/acyl fluorides, and perhydroalkyl sulfonic acids, alkanes, and alcohols. Computational and Theoretical Chemistry, 2010, 941, 107-118. | 1.5 | 22 |

| # | Article | IF | Citations |
|---|---|---|---|
| 124 | Experimental and Theoretical Conformational Analysis of 5â€Benzylimidazolidinâ€4â€one Derivatives â€“ a â€˜Playgroundâ€™ for Studying Dispersion Interactions and a â€˜Windshieldâ€Wiperâ€™ Effect in Organocatalysis. Helvetica Chimica Acta, 2010, 93, 1-16. | 1.0 | 59 |
| 125 | Assessment of density functionals with longâ€range and/or empirical dispersion corrections for conformational energy calculations of peptides. Journal of Computational Chemistry, 2010, 31, 2915-2923. | 1.5 | 46 |
| 126 | Anionic d<sup>8</sup> Alkyl Hydrides â€“ Selective Formation and Reactivity of Anionic cisâ€Pt<sup>II</sup> Methyl Hydride. European Journal of Inorganic Chemistry, 2010, 2010, 1991-1999. | 1.0 | 7 |
| 127 | Copperâ€Catalyzed Enantioselective [2+2]â€‰Cycloadditions of 2â€Nitrosopyridine with Ketenes. Advanced Synthesis and Catalysis, 2010, 352, 945-948. | 2.1 | 43 |
| 128 | Effect of CO on the Oxidative Addition of Arene Cï£¿H Bonds by Cationic Rhodium Complexes. Chemistry - A European Journal, 2010, 16, 328-353. | 1.7 | 49 |
| 129 | Labdane diterpenoids and highly methoxylated bibenzyls from the liverwort Frullania inouei. Phytochemistry, 2010, 71, 1573-1578. | 1.4 | 23 |
| 130 | Assessment of density functionals for predicting the infrared spectrum of sodiated octa-glycine. International Journal of Mass Spectrometry, 2010, 297, 152-161. | 0.7 | 21 |
| 131 | A performance study of density functional theory with empirical dispersion corrections and spin-component scaled second-order MÃ¸llerâ^'Plesset perturbation theory on adsorbateâ€“zeolite interactions. Computational and Theoretical Chemistry, 2010, 945, 85-88. | 1.5 | 13 |
| 132 | Gas phase isomerization enthalpies of organic compounds: A semiempirical, density functional theory, and ab initio post-Hartreeâ€“Fock theoretical study. Computational and Theoretical Chemistry, 2010, 948, 102-107. | 1.5 | 50 |
| 133 | Hydrogen bonding interactions in cysteineâ€“urea complexes: Theoretical studies of structures, properties and topologies. Computational and Theoretical Chemistry, 2010, 960, 98-105. | 1.5 | 10 |
| 134 | Metal induced amino acid adsorption on nanotubes. Thin Solid Films, 2010, 518, 2070-2076. | 0.8 | 16 |
| 135 | On the geometrical structure and spectral properties of pyrene monomer and sterically constrained intramolecular pyrene dimers. Chemical Physics, 2010, 377, 123-131. | 0.9 | 9 |
| 136 | Comparative theoretical investigation on the isomerization energies of long-chain perfluoroalkanes: A case study with perfluorooctane sulfonic acid congeners. Nature Precedings, 2010, , . | 0.1 | 0 |
| 137 | The Aromatic Amino Acid Hydroxylase Mechanism: A Perspective From Computational Chemistry. Advances in Inorganic Chemistry, 2010, , 437-500. | 0.4 | 11 |
| 138 | XYG3s: Speedup of the XYG3 fifth-rung density functional with scaling-all-correlation method. Journal of Chemical Physics, 2010, 132, 194105. | 1.2 | 40 |
| 139 | Basis set consistent revision of the S22 test set of noncovalent interaction energies. Journal of Chemical Physics, 2010, 132, 144104. | 1.2 | 309 |
| 140 | The assessment of density functionals for DNAâ€“protein stacked and T-shaped complexes. Canadian Journal of Chemistry, 2010, 88, 815-830. | 0.6 | 36 |
| 141 | Basis set dependence of the doubly hybrid XYG3 functional. Journal of Chemical Physics, 2010, 133, 104105. | 1.2 | 41 |

| # | Article | IF | Citations |
|---|---|---|---|
| 142 | Intriguing Ï€<sup>+</sup>â^'Ï€ Interaction in Crystal Packing. Journal of Physical Chemistry B, 2010, 114, 4166-4170. | 1.2 | 55 |
| 143 | Probing Substituent Effects in Arylâ^'Aryl Interactions Using Stereoselective Dielsâ^'Alder Cycloadditions. Journal of the American Chemical Society, 2010, 132, 3304-3311. | 6.6 | 176 |
| 144 | Significant van der Waals Effects in Transition Metal Complexes. Journal of Chemical Theory and Computation, 2010, 6, 2040-2044. | 2.3 | 185 |
| 145 | Extending the reliability and applicability of B3LYP. Chemical Communications, 2010, 46, 3057. | 2.2 | 196 |
| 146 | Using Nonempirical Semilocal Density Functionals and Empirical Dispersion Corrections to Model Dative Bonding in Substituted Boranes. Journal of Chemical Theory and Computation, 2010, 6, 1825-1833. | 2.3 | 22 |
| 147 | Formation and structure of the potassium complex of valinomycin in solution studied by Raman optical activity spectroscopy. Physical Chemistry Chemical Physics, 2010, 12, 11021. | 1.3 | 57 |
| 148 | A General Database for Main Group Thermochemistry, Kinetics, and Noncovalent Interactions â^' Assessment of Common and Reparameterized (meta-)GGA Density Functionals. Journal of Chemical Theory and Computation, 2010, 6, 107-126. | 2.3 | 389 |
| 149 | Using Density Functional Theory Methods for Modeling Induction and Dispersion Interactions in Ligandâ€"Protein Complexes. Annual Reports in Computational Chemistry, 2010, 6, 96-112. | 0.9 | 6 |
| 150 | van der Waals Interactions in Density-Functional Theory: Intermolecular Complexes. Journal of Chemical Theory and Computation, 2010, 6, 1081-1088. | 2.3 | 155 |
| 151 | Branched Alkanes Have Contrasting Stabilities. Organic Letters, 2010, 12, 3070-3073. | 2.4 | 34 |
| 152 | Synthesis and Structure of m-Terphenyl Thio-, Seleno-, and Telluroethers. Journal of Organic Chemistry, 2010, 75, 8363-8371. | 1.7 | 17 |
| 153 | A New Empirical Correction to the AM1 Method for Macromolecular Complexes. Journal of Chemical Theory and Computation, 2010, 6, 2153-2166. | 2.3 | 23 |
| 154 | Effects of London dispersion on the isomerization reactions of large organic molecules: a density functional benchmark study. Physical Chemistry Chemical Physics, 2010, 12, 6940. | 1.3 | 123 |
| 155 | Accurately Characterizing the Ï€â^'Ï€ Interaction Energies of Indoleâ^'Benzene Complexes. Journal of Physical Chemistry A, 2010, 114, 3576-3582. | 1.1 | 63 |
| 156 | Ï€ Interactions Studied with Electronic Structure Methods: The Ethyne Methyl Isocyanide Complex and Thioanisole. Journal of Chemical Theory and Computation, 2010, 6, 2687-2700. | 2.3 | 7 |
| 157 | Synthesis and Reactivity of an Iridium(I) Acetonyl PNP Complex. Experimental and Computational Study of Metalâ^'Ligand Cooperation in Hâ^'H and Câ^'H Bond Activation via Reversible Ligand Dearomatization. Organometallics, 2010, 29, 3817-3827. | 1.1 | 97 |
| 158 | Conformational Preferences of X-Pro Sequences: Ala-Pro and Aib-Pro Motifs. Journal of Physical Chemistry B, 2010, 114, 14077-14086. | 1.2 | 10 |
| 159 | Intramolecular Proton Transfer in Calixphyrin Derivatives. Journal of Physical Chemistry A, 2010, 114, 3649-3654. | 1.1 | 6 |

| # | Article | IF | Citations |
|---|---|---|---|
| 160 | Intramolecular Ï€âˆ'Ï€ Stacking Interactions in 2-Substituted N,N-Dibenzylaziridinium Ions and Their Regioselectivity in Nucleophilic Ring-Opening Reactions. Journal of Organic Chemistry, 2010, 75, 885-896. | 1.7 | 66 |
| 161 | A Theoretical Study of Brominated Porphycenes: Electronic Spectra and Intersystem Spinâˆ'Orbit Coupling. Journal of Chemical Theory and Computation, 2010, 6, 3176-3189. | 2.3 | 21 |
| 162 | Effect of Charge Distribution on RDX Adsorption in IRMOF-10. Langmuir, 2010, 26, 5942-5950. | 1.6 | 27 |
| 163 | On the Free Radical Scavenging Capability of Carboxylated Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 6363-6370. | 1.5 | 32 |
| 164 | An Assessment of Density Functional Methods for Potential Energy Curves of Nonbonded Interactions: The XYG3 and B97-D Approximations. Journal of Chemical Theory and Computation, 2010, 6, 727-734. | 2.3 | 91 |
| 165 | A System-Dependent Density-Based Dispersion Correction. Journal of Chemical Theory and Computation, 2010, 6, 1990-2001. | 2.3 | 133 |
| 166 | Trends in Râˆ'X Bond Dissociation Energies (Râ€¢ = Me, Et, i-Pr, t-Bu, Xâ€¢ = H, Me, Cl, OH). Journal of Chemical Theory and Computation, 2010, 6, 1462-1469. | 2.3 | 39 |
| 167 | Stabilization and Structure Calculations for Noncovalent Interactions in Extended Molecular Systems Based on Wave Function and Density Functional Theories. Chemical Reviews, 2010, 110, 5023-5063. | 23.0 | 697 |
| 168 | Thermochemical benchmarking of hydrocarbon bond separation reaction energies: Jacob's ladder is not reversed!. Molecular Physics, 2010, 108, 2655-2666. | 0.8 | 53 |
| 169 | DSD-BLYP: A General Purpose Double Hybrid Density Functional Including Spin Component Scaling and Dispersion Correction. Journal of Physical Chemistry C, 2010, 114, 20801-20808. | 1.5 | 329 |
| 170 | Theoretical Investigation of the Rubicordifolin Cascade. Organic Letters, 2010, 12, 5162-5165. | 2.4 | 20 |
| 171 | Empirically corrected DFT and semi-empirical methods for non-bonding interactions. Physical Chemistry Chemical Physics, 2010, 12, 307-322. | 1.3 | 77 |
| 172 | Frontiers in electronic structure theory. Journal of Chemical Physics, 2010, 132, 110902. | 1.2 | 147 |
| 173 | Van der Waals Interaction between Two Crossed Carbon Nanotubes. ACS Nano, 2010, 4, 5937-5945. | 7.3 | 98 |
| 174 | The [13]Annulene Cation Is a Stable MÃ¶bius Annulene Cation. Organic Letters, 2010, 12, 1708-1711. | 2.4 | 24 |
| 175 | Harmonic and Anharmonic Vibrational Frequency Calculations with the Double-Hybrid B2PLYP Method: Analytic Second Derivatives and Benchmark Studies. Journal of Chemical Theory and Computation, 2010, 6, 2115-2125. | 2.3 | 274 |
| 176 | Modeling the noble metal/TiO2 (110) interface with hybrid DFT functionals: A periodic electrostatic embedded cluster model study. Journal of Chemical Physics, 2010, 133, 164703. | 1.2 | 59 |
| 177 | Theoretical Study of the Hydrolysis of Pentameric Aluminum Complexes. Journal of Chemical Theory and Computation, 2010, 6, 993-1007. | 2.3 | 18 |

| # | Article | IF | Citations |
|---|---|---|---|
| 178 | Structure of the gas-phase glycine tripeptide. Physical Chemistry Chemical Physics, 2010, 12, 3463. | 1.3 | 22 |
| 179 | DFT Study of the Structure and Reactivity of the Terminal Pt(IV)-Oxo Complex Bearing No Electron-Withdrawing Ligands. Journal of the American Chemical Society, 2010, 132, 14886-14900. | 6.6 | 49 |
| 180 | Doubly hybrid density functional for accurate description of thermochemistry, thermochemical kinetics and nonbonded interactions. International Reviews in Physical Chemistry, 2011, 30, 115-160. | 0.9 | 116 |
| 181 | Thermal Câ^'H Bond Activation of Benzene, Toluene, and Methane with Cationic [M(X)(bipy)]+(M = Ni, Pd,) Tj ETQq1 1 0.784314 rgBT | 1.1 | 46 |
| 182 | Ring-opening radical clock reactions: many density functionals have difficulty keeping time. Organic and Biomolecular Chemistry, 2011, 9, 3158. | 1.5 | 5 |
| 183 | Vibrations of a chelated proton in a protonated tertiary diamine. Physical Chemistry Chemical Physics, 2011, 13, 20380. | 1.3 | 15 |
| 184 | Theoretical investigation of the complexation of crown ethers and crown ethers of fulleropyrrolidine with (CH<sub>3</sub>)<sub>x</sub>NH+4â^'x, x = 0â€“4. Physical Chemistry Chemical Physics, 2011, 13, 954-965. | 1.3 | 10 |
| 185 | Bonding Nature and Vibrational Signatures of Oxirane:(Water)<sub>n=1â€“3</sub>. Assessment of the Performance of the Dispersion-Corrected DFT Methods Compared to the ab initio Results and Fourier Transform Infrared Experimental Data. Journal of Physical Chemistry A, 2011, 115, 6688-6701. | 1.1 | 12 |
| 186 | Energy and Lifetime of Temporary Anion States of Uracil by Stabilization Method. Journal of Physical Chemistry A, 2011, 115, 10113-10121. | 1.1 | 23 |
| 187 | Direct Infrared Absorption Spectroscopy of Benzene Dimer. Journal of Physical Chemistry A, 2011, 115, 11263-11268. | 1.1 | 36 |
| 188 | Ab Initio Modeling of Donorâ€“Acceptor Interactions and Charge-Transfer Excitations in Molecular Complexes: The Case of Terthiopheneâ€“Tetracyanoquinodimethane. Journal of Chemical Theory and Computation, 2011, 7, 2068-2077. | 2.3 | 46 |
| 189 | Solvation Effects on Electronic Transitions: Exploring the Performance of Advanced Solvent Potentials in Polarizable Embedding Calculations. Journal of Chemical Theory and Computation, 2011, 7, 2209-2217. | 2.3 | 75 |
| 190 | Density Functional Study of the Stable Oxidation States and the Binding of Oxygen in MO<sub>4</sub> Clusters of the 3d Elements. Journal of Physical Chemistry A, 2011, 115, 10665-10678. | 1.1 | 21 |
| 191 | Cyclization Reactions of 3,4-Diazaheptatrienyl Metal Compounds. Pyridines from an Anionic Analogue of the Fischer Indole Synthesis: Experiment and Theory. Journal of Organic Chemistry, 2011, 76, 4591-4599. | 1.7 | 18 |
| 192 | Protonation of Phosphovanadomolybdates H<sub>3+x</sub>PV<sub>x</sub>Mo<sub>12â€“x</sub>O<sub>40</sub>: Computational Insight Into Reactivity. Journal of Physical Chemistry A, 2011, 115, 4811-4826. | 1.1 | 40 |
| 193 | Assessment of Dispersion Corrected Atom Centered Pseudopotentials: Application to Energetic Molecular Crystals. Journal of Physical Chemistry B, 2011, 115, 803-810. | 1.2 | 32 |
| 194 | Dimer Radical Cations of Indole and Indole-3-carbinol: Localized and Delocalized Radical Cations of Diindolylmethane. Journal of Physical Chemistry A, 2011, 115, 7700-7708. | 1.1 | 8 |
| 195 | Theoretical Studies on Thermochemistry for Conversion of 5-Chloromethylfurfural into Valuable Chemicals. Journal of Physical Chemistry A, 2011, 115, 13628-13641. | 1.1 | 25 |

| # | Article | IF | Citations |
|---|---|---|---|
| 196 | Explicitly Correlated Coupled Cluster Calculations for the Benzenium Ion (C<sub>6</sub>H<sub>7</sub><sup>+</sup>) and Its Complexes with Ne and Ar. Journal of Physical Chemistry A, 2011, 115, 13664-13672. | 1.1 | 12 |
| 197 | Cationâ"Cation â€œAttractionâ€: When London Dispersion Attraction Wins over Coulomb Repulsion. Inorganic Chemistry, 2011, 50, 2619-2628. | 1.9 | 127 |
| 198 | Transition States and Energetics of Nucleophilic Additions of Thiols to Substituted Î±,Î²-Unsaturated Ketones: Substituent Effects Involve Enone Stabilization, Product Branching, and Solvation. Journal of Organic Chemistry, 2011, 76, 5074-5081. | 1.7 | 84 |
| 199 | Differences in structure, energy, and spectrum between neutral, protonated, and deprotonated phenol dimers: comparison of various density functionals with ab initio theory. Physical Chemistry Chemical Physics, 2011, 13, 991-1001. | 1.3 | 39 |
| 200 | Theoretical Study on the Mechanism of the Oxygen Activation Process in Cysteine Dioxygenase Enzymes. Journal of the American Chemical Society, 2011, 133, 3869-3882. | 6.6 | 197 |
| 201 | Molecular Simulation of the Pressure-Induced Crystallographic Phase Transition of p-Terphenyl. Journal of Physical Chemistry B, 2011, 115, 407-413. | 1.2 | 12 |
| 202 | Understanding the HIV-1 Protease Reactivity with DFT: What Do We Gain from Recent Functionals?. Journal of Physical Chemistry B, 2011, 115, 8545-8558. | 1.2 | 27 |
| 203 | Theoretical Investigation on Triplet Excitation Energy Transfer in Fluorene Dimer. Chinese Journal of Chemical Physics, 2011, 24, 538-546. | 0.6 | 6 |
| 204 | Double-hybrid density-functional theory made rigorous. Journal of Chemical Physics, 2011, 134, 064113. | 1.2 | 165 |
| 205 | Halogen Bond Involving Hypervalent Halogen: CSD Search and Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 9294-9299. | 1.1 | 55 |
| 206 | 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. Journal of Chemical Theory and Computation, 2011, 7, 658-668. | 2.3 | 73 |
| 207 | A Parameter-Free Density Functional That Works for Noncovalent Interactions. Journal of Physical Chemistry Letters, 2011, 2, 983-989. | 2.1 | 134 |
| 209 | Accurate Conformational Energy Differences of Carbohydrates: A Complete Basis Set Extrapolation. Journal of Chemical Theory and Computation, 2011, 7, 988-997. | 2.3 | 26 |
| 210 | Conformational Analysis of a Nitroxide Side Chain in an Î±-Helix with Density Functional Theory. Journal of Physical Chemistry B, 2011, 115, 397-405. | 1.2 | 36 |
| 211 | Quantum Mechanical Modeling of Catalytic Processes. Annual Review of Chemical and Biomolecular Engineering, 2011, 2, 453-477. | 3.3 | 68 |
| 212 | Photoinduced Singlet Charge Transfer in a Ruthenium(II) Perylene-3,4:9,10-bis(dicarboximide) Complex. Journal of Physical Chemistry B, 2011, 115, 7533-7540. | 1.2 | 36 |
| 213 | Accurate Interaction Energies for Problematic Dispersion-Bound Complexes: Homogeneous Dimers of NCCN, P2, and PCCP. Journal of Chemical Theory and Computation, 2011, 7, 2842-2851. | 2.3 | 46 |
| 214 | Hybrid Quantum and Classical Simulations of the Dihydrofolate Reductase Catalyzed Hydride Transfer Reaction on an Accurate Semi-Empirical Potential Energy Surface. Journal of Chemical Theory and Computation, 2011, 7, 3420-3437. | 2.3 | 45 |

| # | Article | IF | Citations |
|---|---|---|---|
| 215 | Geometry of (E)-benzaldehyde phenylhydrazone in ethanol. Computational and Theoretical Chemistry, 2011, 976, 197-200. | 1.1 | 0 |
| 216 | Singletâ€“triplet (S0â†'T1) excitation energies of the [4Ã—n] rectangular graphene nanoribbon series (n=2â€“6): A comparative theoretical study. Computational and Theoretical Chemistry, 2011, 977, 163-167. | 1.1 | 13 |
| 217 | First-principles investigation on the structural stability of methane and ethane clathrate hydrates. Computational and Theoretical Chemistry, 2011, 977, 209-212. | 1.1 | 14 |
| 218 | A comparison between artificial and natural water oxidation. Dalton Transactions, 2011, 40, 11296. | 1.6 | 34 |
| 219 | Efficient and Accurate Double-Hybrid-Meta-GGA Density Functionalsâ€"Evaluation with the Extended GMTKN30 Database for General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2011, 7, 291-309. | 2.3 | 1,035 |
| 220 | Theoretical investigation on quinoline-based platinum (II) complexes as efficient singlet oxygen photosensitizers in photodynamic therapy. Journal of Organometallic Chemistry, 2011, 696, 3322-3327. | 0.8 | 34 |
| 221 | How reliable are DFT transition structures? Comparison of GGA, hybrid-meta-GGA and meta-GGA functionals. Organic and Biomolecular Chemistry, 2011, 9, 689-700. | 1.5 | 212 |
| 222 | Comprehensive Benchmarking of a Density-Dependent Dispersion Correction. Journal of Chemical Theory and Computation, 2011, 7, 3567-3577. | 2.3 | 400 |
| 223 | Semiempirical, Hartree-Fock, density functional, and second order Moller-Plesset perturbation theory methods do not accurately predict ionization energies and electron affinities of short- through long-chain [n]acenes. Nature Precedings, 2011, , . | 0.1 | 1 |
| 224 | Gas phase enthalpies of formation, isomerization, and disproportionation of mono- through tetra-substituted tetrahedranes: A G4MP2/G4 theoretical study. Nature Precedings, 2011, , . | 0.1 | 0 |
| 225 | An introduction to quantum chemical methods applied to drug design. Frontiers in Bioscience - Elite, 2011, E3, 1061-1078. | 0.9 | 0 |
| 226 | Seeking for parameter-free double-hybrid functionals: The PBE0-DH model. Journal of Chemical Physics, 2011, 135, 024106. | 1.2 | 226 |
| 227 | A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. Physical Chemistry Chemical Physics, 2011, 13, 6670. | 1.3 | 1,627 |
| 228 | Confinement Effect on p-Nitroaniline Electronic Spectrum and Electric Properties. Journal of Physical Chemistry A, 2011, 115, 5210-5220. | 1.1 | 18 |
| 229 | Density-functional approaches to noncovalent interactions: A comparison of dispersion corrections (DFT-D), exchange-hole dipole moment (XDM) theory, and specialized functionals. Journal of Chemical Physics, 2011, 134, 084107. | 1.2 | 607 |
| 230 | Radicalâ€Transfer Hydroamination of Olefins with Nâ€Aminated Dihydropyridines. Chemistry - an Asian Journal, 2011, 6, 1197-1209. | 1.7 | 52 |
| 231 | Calculations of ionization energies and electron affinities for atoms and molecules: A comparative study with different methods. Frontiers of Chemistry in China: Selected Publications From Chinese Universities, 2011, 6, 269-279. | 0.4 | 22 |
| 232 | Quantum Mechanical Investigations of Organocatalysis: Mechanisms, Reactivities, and Selectivities. Chemical Reviews, 2011, 111, 5042-5137. | 23.0 | 489 |

| # | Article | IF | Citations |
|---|---|---|---|
| 233 | Noncovalent interactions in biochemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 3-17. | 6.2 | 222 |
| 234 | Density Functional Calculations. , 2011, , 445-519. | | 3 |
| 235 | Carbocations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 487-508. | 6.2 | 43 |
| 236 | The quantum chemical cluster approach for modeling enzyme reactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 323-336. | 6.2 | 232 |
| 237 | Density functional theory with London dispersion corrections. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 211-228. | 6.2 | 2,030 |
| 238 | Hydrogen bonding interactions between N,N-dimethylformamide and cysteine: DFT studies of structures, properties, and topologies. Structural Chemistry, 2011, 22, 57-65. | 1.0 | 22 |
| 239 | Hydrogen bonding interactions in noradrenaline-DMSO complexes: DFT and QTAIM studies of structure, properties and topology. Journal of Molecular Modeling, 2011, 17, 2609-2621. | 0.8 | 25 |
| 240 | Microsolvation of aminoethanol: a study using DFT combined with QTAIM. Journal of Molecular Modeling, 2011, 17, 2781-2796. | 0.8 | 14 |
| 241 | Bonding in cationic MOH n + (MÂ=ÂKÂâˆ'ÂLa, HfÂâˆ'ÂRn; nÂ=Â0â€"2): DFT performances and periodic trends. Theoretical Chemistry Accounts, 2011, 129, 389-399. | 0.5 | 40 |
| 242 | Theoretical insights into the catalytic mechanism of Î²-hexosaminidase. Theoretical Chemistry Accounts, 2011, 129, 119-129. | 0.5 | 13 |
| 243 | Advances in local hybrid exchangeâ€"correlation functionals: from thermochemistry to magneticâ€"resonance parameters and hyperpolarizabilities. International Journal of Quantum Chemistry, 2011, 111, 2625-2638. | 1.0 | 42 |
| 244 | Development of force field parameters for oxyluciferin on its electronic ground and excited states. International Journal of Quantum Chemistry, 2011, 111, 4091-4105. | 1.0 | 28 |
| 245 | Substrate Hydroxylation by the Oxidoâ€"Iron Intermediate in Aromatic Amino Acid Hydroxylases: A DFT Mechanistic Study. European Journal of Inorganic Chemistry, 2011, 2011, 2720-2732. | 1.0 | 5 |
| 246 | Validation of DFT-Based Methods for Predicting Qualitative Thermochemistry of Large Polyaromatics. ChemPhysChem, 2011, 12, 1100-1108. | 1.0 | 8 |
| 247 | Compact Folding of Isolated Fourâ€Residue Neutral Peptide Chains: Hâ€Bonding Patterns and Entropy Effects. ChemPhysChem, 2011, 12, 1889-1899. | 1.0 | 45 |
| 248 | Understanding the Influence of Guestâ€"Host Interactions on the Conformation of Short Peptides in a Hydrophobic Cavity: A Computational Study. ChemPhysChem, 2011, 12, 1325-1333. | 1.0 | 2 |
| 249 | The Effect of Backbone Constraints: The Case of Water Oxidation by the Oxygenâ€Evolving Complex in PSII. ChemPhysChem, 2011, 12, 3274-3280. | 1.0 | 90 |
| 250 | Substituent Effects on Nonâ€Covalent Interactions with Aromatic Rings: Insights from Computational Chemistry. ChemPhysChem, 2011, 12, 3116-3130. | 1.0 | 132 |

| # | Article | IF | Citations |
|---|---|---|---|
| 251 | Benchmarking Density Functional Methods against the S66 and S66x8 Datasets for Nonâ€Covalent Interactions. ChemPhysChem, 2011, 12, 3421-3433. | 1.0 | 283 |
| 252 | A comparison of the behavior of functional/basis set combinations for hydrogenâ€bonding in the water dimer with emphasis on basis set superposition error. Journal of Computational Chemistry, 2011, 32, 1519-1527. | 1.5 | 137 |
| 253 | The shape of gaseous nâ€butylbenzene: Assessment of computational methods and comparison with experiments. Journal of Computational Chemistry, 2011, 32, 1550-1560. | 1.5 | 6 |
| 254 | Infinite basis set extrapolation for double hybrid density functional theory 1: Effect of applying various extrapolation functions. Journal of Computational Chemistry, 2011, 32, 1671-1679. | 1.5 | 10 |
| 255 | Accurate bond dissociation enthalpies by using doubly hybrid XYG3 functional. Journal of Computational Chemistry, 2011, 32, 1824-1838. | 1.5 | 26 |
| 256 | Ï€â€“Ï€ interaction of quinacridone derivatives. Journal of Computational Chemistry, 2011, 32, 2055-2063. | 1.5 | 11 |
| 258 | Highly Asymmetric NHCâ€Catalyzed Hydroacylation of Unactivated Alkenes. Angewandte Chemie - International Edition, 2011, 50, 4983-4987. | 7.2 | 186 |
| 259 | Conformational preference and cisâ€“trans isomerization of 4â€methylproline residues. Biopolymers, 2011, 95, 51-61. | 1.2 | 25 |
| 260 | Conformational preferences and pK<sub>a</sub> value of selenocysteine residue. Biopolymers, 2011, 95, 345-353. | 1.2 | 34 |
| 261 | Mechanistic Insight into Stereoselective Carbolithiation. Chemistry - A European Journal, 2011, 17, 2996-3004. | 1.7 | 35 |
| 262 | Can Enantioselectivity be Computed in Enthalpic Barrierless Reactions? The Case of Cu<sup>I</sup>â€Catalyzed Cyclopropanation of Alkenes. Chemistry - A European Journal, 2011, 17, 529-539. | 1.7 | 14 |
| 263 | Formation of the Ironâ€“Oxo Hydroxylating Species in the Catalytic Cycle of Aromatic Amino Acid Hydroxylases. Chemistry - A European Journal, 2011, 17, 3746-3758. | 1.7 | 12 |
| 264 | Competitive Reactions of Organophosphorus Radicals on Coke Surfaces. Chemistry - A European Journal, 2011, 17, 12027-12036. | 1.7 | 23 |
| 265 | Broken-symmetry natural orbital (BSNO)â€“Mk-MRCC study on the exchange coupling in the binuclear copper(II) compounds. Chemical Physics Letters, 2011, 505, 11-15. | 1.2 | 20 |
| 266 | Recent theoretical studies of water oxidation in photosystem II. Journal of Photochemistry and Photobiology B: Biology, 2011, 104, 94-99. | 1.7 | 92 |
| 267 | Three-component conformational equilibria of some flexible pyrrolidin-2-(thi)ones in solution by NMR data (Î´C, Î´H, and nJHH) and their DFT predictions: a confrontation of different approaches. Tetrahedron, 2011, 67, 6901-6916. | 1.0 | 16 |
| 268 | Theoretical study on the gas and solution phase enthalpies, free energies and equilibrium constants for the isomerisation of [1.1]paracyclophane derivatives as potential molecular switches. Molecular Simulation, 2011, 37, 369-378. | 0.9 | 0 |
| 269 | A fast doubly hybrid density functional method close to chemical accuracy using a local opposite spin ansatz. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 19896-19900. | 3.3 | 143 |

| # | Article | IF | Citations |
|---|---|---|---|
| 270 | A novel relationship between the radical-scavenging activity of flavonoids and enthalpy of formation revealed with Hartreeâ€“Fock computations and thermochemical deduction. Redox Report, 2012, 17, 115-130. | 1.4 | 8 |
| 271 | Long-range corrected hybrid meta-generalized-gradient approximations with dispersion corrections. Journal of Chemical Physics, 2012, 136, 154109. | 1.2 | 101 |
| 272 | B2-PPW91: A promising double-hybrid density functional for the electric response properties. Journal of Chemical Physics, 2012, 136, 124111. | 1.2 | 30 |
| 273 | Complexes of type C6H7+Â·L (L = N2 and CO2) studied by explicitly correlated coupled cluster theory. Journal of Chemical Physics, 2012, 136, 204301. | 1.2 | 2 |
| 274 | Basis set convergence of molecular correlation energy differences within the random phase approximation. Journal of Chemical Physics, 2012, 136, 084105. | 1.2 | 92 |
| 275 | Ab initio calculation of ionization potential and electron affinity of six common explosive compounds. Reports in Theoretical Chemistry, 0, , 11. | 0.0 | 31 |
| 276 | 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 |
| 277 | Spin Multiplicity and Symmetry Breaking in Vanadium-Benzene Complexes. Physical Review Letters, 2012, 109, 053001. | 2.9 | 32 |
| 278 | van der Waals Interaction Energies of Small Fragments of P, As, Sb, S, Se, and Te: Comparison of Complete Basis Set Limit CCSD(T) and DFT with Approximate Dispersion. Journal of Chemical Theory and Computation, 2012, 8, 2301-2309. | 2.3 | 6 |
| 279 | Reliable Quantum Chemical Prediction of the Localized/Delocalized Character of Organic Mixed-Valence Radical Anions. From Continuum Solvent Models to Direct-COSMO-RS. Journal of Chemical Theory and Computation, 2012, 8, 4189-4203. | 2.3 | 83 |
| 280 | Computational Insight into the Initial Steps of the Marsâ€“van Krevelen Mechanism: Electron Transfer and Surface Defects in the Reduction of Polyoxometalates. Journal of the American Chemical Society, 2012, 134, 20669-20680. | 6.6 | 54 |
| 281 | Structures and lattice energies of molecular crystals using density functional theory: Assessment of a local atomic potential approach. Chemical Physics Letters, 2012, 550, 94-98. | 1.2 | 22 |
| 282 | Role of Hydrogen Bonds in Ionic-Liquid-Mediated Extraction of Natural Bioactive Homologues. Industrial & Engineering Chemistry Research, 2012, 51, 5299-5308. | 1.8 | 29 |
| 283 | Generation of Weakly Bound Alâ€“N Lewis Pairs by Hydroalumination of Ynamines and the Activation of Small Molecules: Phenylethyne and Dicyclohexylcarbodiimide. Organometallics, 2012, 31, 3272-3283. | 1.1 | 70 |
| 284 | Quenching of magnetism in hexagonal graphene nanoflakes by non-local electron correlation. Chemical Physics Letters, 2012, 553, 6-10. | 1.2 | 20 |
| 285 | Rearrangement from the heteroantiaromatic borole to the heteroaromatic azaborine motif. Chemical Communications, 2012, 48, 4564. | 2.2 | 42 |
| 286 | The interaction of His337 with the Mn4Ca cluster of photosystem II. Physical Chemistry Chemical Physics, 2012, 14, 4651. | 1.3 | 32 |
| 287 | Fulvenallenyl Cation (C7H5+) and Its Complex with an Argon Atom: Results of High-Level Quantum-Chemical Calculations. Journal of Physical Chemistry A, 2012, 116, 3448-3453. | 1.1 | 2 |

| # | Article | IF | Citations |
|---|---|---|---|
| 288 | Assessment of density functional theory for bonds formed between rare gases and open-shell atoms: a computational study of small molecules containing He, Ar, Kr and Xe. Physical Chemistry Chemical Physics, 2012, 14, 553-561. | 1.3 | 10 |
| 289 | Gas-Phase Reactivity of Group 11 Dimethylmetallates with Allyl Iodide. Journal of the American Chemical Society, 2012, 134, 2569-2580. | 6.6 | 48 |
| 290 | Energies and Lifetimes of Temporary Anion States of Chloromethanes by Stabilized Koopmansâ€™ Theorem in Long-Range Corrected Density Functional Theory. Journal of Physical Chemistry A, 2012, 116, 12364-12372. | 1.1 | 8 |
| 291 | Mechanism for N<sub>2</sub>O Generation in Bacterial Nitric Oxide Reductase: A Quantum Chemical Study. Biochemistry, 2012, 51, 5173-5186. | 1.2 | 81 |
| 292 | Electronic Structure and Reactivity of Cobalt Oxide Dimers and Their Hexacarbonyl Complexes: A Density Functional Study. Journal of Physical Chemistry A, 2012, 116, 3295-3303. | 1.1 | 12 |
| 293 | Theoretical Prediction of Tripletâ€“Triplet Energy Transfer Rates in a Benzophenoneâ€“Fluoreneâ€“Naphthalene System. Journal of Physical Chemistry C, 2012, 116, 12499-12507. | 1.5 | 14 |
| 294 | Unraveling the Mechanisms of Carboxyl Ester Bond Hydrolysis Catalyzed by a Vanadate Anion. Inorganic Chemistry, 2012, 51, 9619-9628. | 1.9 | 7 |
| 295 | Improving Predictions of Gas Adsorption in Metalâ€“Organic Frameworks with Coordinatively Unsaturated Metal Sites: Model Potentials, ab initio Parameterization, and GCMC Simulations. Journal of Physical Chemistry C, 2012, 116, 18899-18909. | 1.5 | 102 |
| 296 | Exploring the Limits of Density Functional Approximations for Interaction Energies of Molecular Precursors to Organic Electronics. Journal of Chemical Theory and Computation, 2012, 8, 4305-4316. | 2.3 | 38 |
| 297 | Isomerization energies of tetrahedranes to 1,3-cyclobutadienes: A challenge for theoretical methods. Computational and Theoretical Chemistry, 2012, 979, 1-9. | 1.1 | 8 |
| 298 | Self-consistent addition of an atomic charge dependent hydrogen-bonding correction function. Computational and Theoretical Chemistry, 2012, 984, 9-12. | 1.1 | 3 |
| 299 | Singletâ€“triplet excitation energies of naphthyl cations: High level composite method calculations suggest a singlet ground state. Computational and Theoretical Chemistry, 2012, 983, 69-75. | 1.1 | 9 |
| 300 | Thioformyl chloride dimer: An excellent model system for the assessment of new computational methods. Computational and Theoretical Chemistry, 2012, 983, 83-87. | 1.1 | 2 |
| 301 | Quantum chemical and theoretical kinetics studies on the reaction of carbonyl sulfide with H, OH and O(3P). Computational and Theoretical Chemistry, 2012, 994, 25-33. | 1.1 | 20 |
| 302 | Comparison of some dispersion-corrected and traditional functionals with CCSD(T) and MP2 ab initio methods: Dispersion, induction, and basis set superposition error. Journal of Chemical Physics, 2012, 137, 134109. | 1.2 | 49 |
| 303 | Perspective: Advances and challenges in treating van der Waals dispersion forces in density functional theory. Journal of Chemical Physics, 2012, 137, 120901. | 1.2 | 931 |
| 304 | A high level computational study of the CH<sub>4</sub>/CF<sub>4</sub>dimer: how does it compare with the CH<sub>4</sub>/CH<sub>4</sub>and CF<sub>4</sub>/CF<sub>4</sub>dimers?. Molecular Physics, 2012, 110, 377-387. | 0.8 | 21 |
| 305 | A Computational Study of Semiconducting Benzobisthiazoles: Analysis of the Substituent Effects on the Electronic Structure, Solid-State Interactions, and Charge Transport Properties Using DFT Methods. Journal of Physical Chemistry C, 2012, 116, 22663-22674. | 1.5 | 13 |

| # | Article | IF | Citations |
|---|---|---|---|
| 306 | Adsorption of Hydrocarbons in Metalâ€“Organic Frameworks: A Force Field Benchmark on the Example of Benzene in Metalâ€“Organic Framework 5. Journal of Physical Chemistry C, 2012, 116, 15369-15377. | 1.5 | 14 |
| 307 | XYG3 and XYGJ-OS performances for noncovalent binding energies relevant to biomolecular structures. Physical Chemistry Chemical Physics, 2012, 14, 12554. | 1.3 | 32 |
| 308 | Characterization of the Temporary Anion States on Perfluoroalkanes via Stabilized Koopmansâ€™ Theorem in Long-Range Corrected Density Functional Theory. Journal of Physical Chemistry A, 2012, 116, 3224-3236. | 1.1 | 12 |
| 309 | A pass too far: dissociation of internal energy selected paracyclophane cations, theory and experiment. Physical Chemistry Chemical Physics, 2012, 14, 11920. | 1.3 | 17 |
| 310 | Exclusive Câ€“C Oxidative Addition in a Rhodium Thiophosphoryl Pincer Complex and Computational Evidence for an Î·<sup>3</sup>-Câ€“Câ€“H Agostic Intermediate. Organometallics, 2012, 31, 505-512. | 1.1 | 33 |
| 311 | Can two T-shaped isomers of OCSâ€“C2H2 van der Waals complex exist?. Chemical Physics Letters, 2012, 549, 6-11. | 1.2 | 16 |
| 312 | Investigating inclusion complexes using quantum chemical methods. Chemical Society Reviews, 2012, 41, 3119. | 18.7 | 60 |
| 313 | Advancing Understanding and Design of Functional Materials Through Theoretical and Computational Chemical Physics. , 2012, , 209-278. | | 3 |
| 314 | Practical Aspects of Computational Chemistry II. , 2012, , . | | 2 |
| 315 | Explicitly correlated benchmark calculations on C<sub>8</sub>H<sub>8</sub> isomer energy separations: how accurate are DFT, double-hybrid, and composite ab initio procedures?. Molecular Physics, 2012, 110, 2477-2491. | 0.8 | 63 |
| 316 | Kinetic (T = 201â€“298 K) and Equilibrium (T = 320â€“420 K) Measurements of the C3H5 + O2 â‡† C3H5O2 Reaction. Journal of Physical Chemistry A, 2012, 116, 3969-3978. | 1.1 | 19 |
| 317 | Noncovalent Interactions in SIESTA Using the vdW-DF Functional: S22 Benchmark and Macrocyclic Structures. Journal of Chemical Theory and Computation, 2012, 8, 281-289. | 2.3 | 26 |
| 318 | Dimethylcuprate-Catalyzed Decarboxylative Coupling of Allyl Acetate. Organometallics, 2012, 31, 8012-8023. | 1.1 | 27 |
| 319 | Mechanisms for proton release during water oxidation in the S2 to S3 and S3 to S4 transitions in photosystem II. Physical Chemistry Chemical Physics, 2012, 14, 4849. | 1.3 | 149 |
| 320 | Modelling the metal atom positions of the Photosystem II water oxidising complex: a density functional theory appraisal of the 1.9 Ã… resolution crystal structure. Physical Chemistry Chemical Physics, 2012, 14, 11333. | 1.3 | 50 |
| 321 | Improving density functional theory for crystal polymorph energetics. Physical Chemistry Chemical Physics, 2012, 14, 7739. | 1.3 | 32 |
| 322 | Recent trends in conformational analysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 613-641. | 6.2 | 65 |
| 323 | Synthesis and rotation barriers in 2, 6â€Diâ€(oâ€anisyl) anisole. Journal of Physical Organic Chemistry, 2012, 25, 878-882. | 0.9 | 2 |

| # | Article | IF | Citations |
|---|---|---|---|
| 324 | Can computational approaches aid in untangling the inherent complexity of practical organic photovoltaic systems?. Journal of Polymer Science, Part B: Polymer Physics, 2012, 50, 1071-1089. | 2.4 | 29 |
| 325 | A theoretical study of Nâ€“Hâ€‰Â·Â·Â·â€‰Ï€ H-bond interaction of pyrrole: from clusters to the liquid. Molecular Physics, 2012, 110, 2151-2161. | 0.8 | 6 |
| 326 | Correlations between Computation and Experimental Thermodynamics of Halogen Bonding. Journal of Organic Chemistry, 2012, 77, 3483-3491. | 1.7 | 90 |
| 327 | Fluorescence Lifetimes and Quantum Yields of Rhodamine Derivatives: New Insights from Theory and Experiment. Journal of Physical Chemistry A, 2012, 116, 7491-7497. | 1.1 | 108 |
| 328 | An Asymmetric Organocatalytic Povarov Reaction with 2-Hydroxystyrenes. Journal of Organic Chemistry, 2012, 77, 6970-6979. | 1.7 | 102 |
| 329 | M<scp>O</scp>V<scp>I</scp>P<scp>AC</scp>: Vibrational spectroscopy with a robust metaâ€program for massively parallel standard and inverse calculations. Journal of Computational Chemistry, 2012, 33, 2186-2198. | 1.5 | 59 |
| 330 | Accurate and fast treatment of large molecular systems: Assessment of CEPA and pCCSD within the local pair natural orbital approximation. Journal of Computational Chemistry, 2012, 33, 2067-2072. | 1.5 | 12 |
| 331 | Infinite Basis Set Extrapolation for Double Hybrid Density Functional Theory 2: Effect of Adding Diffuse Basis Functions. Journal of the Chinese Chemical Society, 2012, 59, 1094-1103. | 0.8 | 4 |
| 332 | Axial and equatorial ligand effects on biomimetic cysteine dioxygenase model complexes. Organic and Biomolecular Chemistry, 2012, 10, 5401. | 1.5 | 17 |
| 333 | Prereactive Complexes in Chlorination of Benzene, Triazine, and Tetrazine: A Quantum Chemical Study. Journal of Physical Chemistry A, 2012, 116, 1298-1306. | 1.1 | 19 |
| 334 | Understanding Structures and Hydrogen Bonds of Ionic Liquids at the Electronic Level. Journal of Physical Chemistry B, 2012, 116, 1007-1017. | 1.2 | 150 |
| 336 | Heterolytic Outerâ€Sphere Cleavage of H<sub>2</sub> for the Reduction of N<sub>2</sub> in the Coordination Sphere of Transition Metalsâ€”A DFT Study. Angewandte Chemie - International Edition, 2012, 51, 8225-8229. | 7.2 | 14 |
| 337 | Iron Borohydride Pincer Complexes for the Efficient Hydrogenation of Ketones under Mild, Baseâ€Free Conditions: Synthesis and Mechanistic Insight. Chemistry - A European Journal, 2012, 18, 7196-7209. | 1.7 | 180 |
| 338 | From Single Molecule to Crystal: Mapping Out the Conformations of Tartaric Acids and Their Derivatives. ChemPhysChem, 2012, 13, 1500-1506. | 1.0 | 8 |
| 339 | Intermolecular Interactions in Weak Donorâ€“Acceptor Complexes from Symmetryâ€Adapted Perturbation and Coupledâ€Cluster Theory: Tetracyanoethyleneâ€“Benzene and Tetracyanoethyleneâ€“pâ€Xylene. ChemPhysChem, 2012, 13, 2769-2776. | 1.0 | 10 |
| 340 | Three Types of Induced Tryptophan Optical Activity Compared in Model Dipeptides: Theory and Experiment. ChemPhysChem, 2012, 13, 2748-2760. | 1.0 | 18 |
| 341 | Assessment of density functional theory to calculate the phase transition pressure of ice. Physical Chemistry Chemical Physics, 2012, 14, 11484. | 1.3 | 22 |
| 342 | Geometries and Vibrational Frequencies of Small Radicals: Performance of Coupled Cluster and More Approximate Methods. Journal of Chemical Theory and Computation, 2012, 8, 2165-2179. | 2.3 | 42 |

| # | Article | IF | Citations |
|---|---|---|---|
| 343 | Design of a Universal Reversible Bidirectional Current Switch Based on the Fullereneâ€“Phthalocyanine Supramolecular System. Journal of Physical Chemistry A, 2012, 116, 6785-6791. | 1.1 | 24 |
| 344 | A theoretical exploration of unexpected amineâ‹¯Ï€ interactions. Physical Chemistry Chemical Physics, 2012, 14, 10747. | 1.3 | 14 |
| 345 | Accurate thermochemistry from a parameterized coupled-cluster singles and doubles model and a local pair natural orbital based implementation for applications to larger systems. Journal of Chemical Physics, 2012, 136, 064101. | 1.2 | 68 |
| 346 | Density functional theory studies on the Dielsâ€“Alder reaction of [3]dendralene with C60: an attractive approach for functionalization of fullerene. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 8 |
| 347 | DFT investigation of endohedral boron oxide nanocapsules: Encapsulation of He, Ne, Ar, H, N, and Cl atoms. Chemical Physics, 2012, 393, 86-95. | 0.9 | 7 |
| 348 | Density functional theory calculation of refractive indices of liquid-forming silicon oil compounds. Chemical Physics, 2012, 394, 40-45. | 0.9 | 6 |
| 349 | The dispersion correction and weak-hydrogen-bond network in low-frequency vibration of solid-state salicylic acid. Chemical Physics Letters, 2012, 531, 98-104. | 1.2 | 27 |
| 350 | Extending the applicability of the PBE0-DH double-hybrid model to weak interactions. Chemical Physics Letters, 2012, 535, 136-139. | 1.2 | 10 |
| 351 | The mechanism for proton pumping in cytochrome c oxidase from an electrostatic and quantum chemical perspective. Biochimica Et Biophysica Acta - Bioenergetics, 2012, 1817, 495-505. | 0.5 | 58 |
| 352 | Progress and Challenges in the Calculation of Electronic Excited States. ChemPhysChem, 2012, 13, 28-51. | 1.0 | 344 |
| 353 | Electron correlation methods based on the random phase approximation. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 353 |
| 354 | An improved theoretical approach to the empirical corrections of density functional theory. Journal of Computer-Aided Molecular Design, 2012, 26, 199-213. | 1.3 | 2 |
| 355 | Microsolvation effect and hydrogen-bonding pattern of taurine-water TA-(H2O)n (n = 1â€“3) complexes. Journal of Molecular Modeling, 2012, 18, 265-274. | 0.8 | 8 |
| 356 | Aromatic Interactions as Control Elements in Stereoselective Organic Reactions. Accounts of Chemical Research, 2013, 46, 979-989. | 7.6 | 216 |
| 357 | Reactivity of amines with hypochlorous acid: Computational study of steric, electronic, and medium effects. International Journal of Quantum Chemistry, 2013, 113, 881-890. | 1.0 | 14 |
| 358 | Dispersion-corrected Rung 3.5 density functionals. Theoretical Chemistry Accounts, 2013, 132, 1. | 0.5 | 1 |
| 359 | Water oxidation mechanism in photosystem II, including oxidations, proton release pathways, Oâ€•O bond formation and O2 release. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 1003-1019. | 0.5 | 335 |
| 360 | Dynamic 1H NMR spectroscopic study of hindered internal rotation in selected N,N-dialkyl isonicotinamides: an experimental and DFT analysis. Tetrahedron, 2013, 69, 8147-8154. | 1.0 | 17 |

| # | Article | IF | Citations |
|---|---|---|---|
| 361 | A Phosphine-Accelerated Ar<sub>F</sub>â€“Chloride Bond Activation Process by Palladium. Organometallics, 2013, 32, 3074-3082. | 1.1 | 3 |
| 362 | Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for copper complexes. Journal of Computational Chemistry, 2013, 34, 2079-2090. | 1.5 | 38 |
| 363 | Zirconium Hydrazides as Metallanitrene Synthons: Release of Molecular N<sub>2</sub> from a Hydrazinediido Complex Induced by Oxidative Nâ€“N Bond Cleavage. Organometallics, 2013, 32, 3877-3889. | 1.1 | 9 |
| 364 | Synthesis, Structures, and Dearomatization by Deprotonation of Iron Complexes Featuring Bipyridine-based PNN Pincer Ligands. Inorganic Chemistry, 2013, 52, 9636-9649. | 1.9 | 53 |
| 365 | Association reaction between SiH3 and H2O2: a computational study of the reaction mechanism and kinetics. Theoretical Chemistry Accounts, 2013, 132, 1. | 0.5 | 7 |
| 366 | Water Oxidation Mechanism for Synthetic Coâ€“Oxides with Small Nuclearity. Journal of the American Chemical Society, 2013, 135, 13804-13813. | 6.6 | 106 |
| 367 | A successive layer-by-layer assembly of supramolecular frameworks driven by a novel type of face-to-face Ï€+â€“Ï€+ interactions. CrystEngComm, 2013, 15, 7879. | 1.3 | 130 |
| 368 | Synthesis and Ligand Non-Innocence of Thiolate-Ligated (N4S) Iron(II) and Nickel(II) Bis(imino)pyridine Complexes. Inorganic Chemistry, 2013, 52, 10467-10480. | 1.9 | 21 |
| 369 | Half-metallicity of graphene nanoribbons and related systems: a new quantum mechanical El Dorado for nanotechnologies â€¦ or a hype for materials scientists?. Journal of Molecular Modeling, 2013, 19, 2699-2714. | 0.8 | 10 |
| 370 | Critical Test of Some Computational Chemistry Methods for Prediction of Gas-Phase Acidities and Basicities. Journal of Chemical Theory and Computation, 2013, 9, 3947-3958. | 2.3 | 38 |
| 371 | What do the azobenzene oligomer helixes have to do with the Golden Ratio?. Computational and Theoretical Chemistry, 2013, 1014, 13-23. | 1.1 | 2 |
| 372 | Intra- and intermolecular forces dependent main chain conformations of esters of Î±,Î²-dehydroamino acids. Journal of Molecular Structure, 2013, 1047, 229-236. | 1.8 | 12 |
| 373 | Transition polarizability model of induced resonance Raman optical activity. Journal of Computational Chemistry, 2013, 34, 2152-2158. | 1.5 | 23 |
| 374 | Structure and Stability of Zn, Cd, and Hg Atom Doped Golden Fullerene (Au<sub>32</sub>). Journal of Physical Chemistry C, 2013, 117, 18777-18788. | 1.5 | 16 |
| 375 | Water adsorption on a copper formate paddlewheel model of CuBTC: A comparative MP2 and DFT study. Chemical Physics Letters, 2013, 587, 7-13. | 1.2 | 40 |
| 376 | Does Hydrogenâ€Bonding Donation to Manganese(IV)â€“Oxo and Iron(IV)â€“Oxo Oxidants Affect the Oxygenâ€Atom Transfer Ability? A Computational Study. Chemistry - A European Journal, 2013, 19, 4058-4068. | 1.7 | 76 |
| 377 | Activation of Nitriles by Metal Ligand Cooperation. Reversible Formation of Ketimido- and Enamido-Rhenium PNP Pincer Complexes and Relevance to Catalytic Design. Journal of the American Chemical Society, 2013, 135, 17004-17018. | 6.6 | 110 |
| 378 | Polarization response of methane encapsulated in water cages. Computational and Theoretical Chemistry, 2013, 1013, 52-56. | 1.1 | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 379 | Economical and Accurate Protocol for Calculating Hydrogen-Bond-Acceptor Strengths. Journal of Chemical Information and Modeling, 2013, 53, 3262-3272. | 2.5 | 14 |
| 380 | A scaling PNOâ€“MP2 method using a hybrid OSVâ€“PNO approach with an iterative direct generation of OSVs<sup>â€</sup>. Molecular Physics, 2013, 111, 2463-2476. | 0.8 | 60 |
| 381 | Accurate non-covalent interactions with basis-set corrections from interference-corrected perturbation theory: comparison with the S22B database. Molecular Physics, 2013, 111, 2299-2305. | 0.8 | 15 |
| 382 | Gas storage of simple molecules in boron oxide nanocapsules. International Journal of Quantum Chemistry, 2013, , n/a-n/a. | 1.0 | 1 |
| 383 | Enhancement in the Stability of 36-Atom Fullerene through Encapsulation of a Uranium Atom. Journal of Physical Chemistry C, 2013, 117, 17859-17869. | 1.5 | 24 |
| 384 | Ru(0) and Ru(II) Nitrosyl Pincer Complexes: Structure, Reactivity, and Catalytic Activity. Inorganic Chemistry, 2013, 52, 11469-11479. | 1.9 | 29 |
| 385 | Unexpected strong stacking interactions between the homogeneous dimers of C6FxI(6â˜x) (x=0, 1, 2, 3, 4) Tj ETQq0 0 0 rgBT /Overlock | 1.1 | 12 |
| 386 | Double-hybrid density functionals: merging wavefunction and density approaches to get the best of both worlds. Physical Chemistry Chemical Physics, 2013, 15, 14581. | 1.3 | 100 |
| 387 | Intramolecular CH/Ï€ interactions in alkylaromatics: Monomer conformations for poly(3â€alkylthiophene) atomistic models. International Journal of Quantum Chemistry, 2013, 113, 2154-2162. | 1.0 | 31 |
| 388 | A mechanistic study supports a two-step mechanism for peptide bond formation on the ribosome. Physical Chemistry Chemical Physics, 2013, 15, 14931. | 1.3 | 11 |
| 389 | Conformational control of benzophenone-sensitized charge transfer in dinucleotides. Physical Chemistry Chemical Physics, 2013, 15, 18607. | 1.3 | 12 |
| 390 | Aromatic Excimers: Ab Initio and TD-DFT Study. Journal of Chemical Theory and Computation, 2013, 9, 847-856. | 2.3 | 57 |
| 391 | Analysis of the performance of DFT-D, M05-2X and M06-2X functionals for studying Ï€â‹¯Ï€ interactions. Chemical Physics Letters, 2013, 557, 170-175. | 1.2 | 77 |
| 392 | From clusters to liquid: what are the preferred ways for benzene and pyrrole to interact?. Theoretical Chemistry Accounts, 2013, 132, 1. | 0.5 | 4 |
| 393 | Critical Evaluation of Implicit Solvent Models for Predicting Aqueous Oxidation Potentials of Neutral Organic Compounds. Journal of Chemical Theory and Computation, 2013, 9, 5046-5058. | 2.3 | 105 |
| 394 | Assessment of Density Functional Theory for Thermochemical Approaches Based on Bond Separation Reactions. Journal of Physical Chemistry A, 2013, 117, 228-243. | 1.1 | 16 |
| 395 | Rationalization of the Barrier Height for p-Z-styrene Epoxidation by Iron(IV)-Oxo Porphyrin Cation Radicals with Variable Axial Ligands. Inorganic Chemistry, 2013, 52, 7968-7979. | 1.9 | 66 |
| 396 | Thermodynamic properties of carbon dioxide clusters by M06-2X and dispersion-corrected B2PLYP-D theory. Chemical Physics Letters, 2013, 573, 19-23. | 1.2 | 30 |

| # | Article | IF | Citations |
|---|---|---|---|
| 397 | Analysis of double-hybrid density functionals along the adiabatic connection. Molecular Physics, 2013, 111, 1275-1294. | 0.8 | 42 |
| 398 | Molecular architecture using novel types of non-covalent Ï€-interactions involving aromatic neutrals, aromatic cations and Ï€-anions. CrystEngComm, 2013, 15, 1285. | 1.3 | 136 |
| 399 | Photophysical properties of azaboradibenzo[6]helicene derivatives. Journal of Materials Chemistry C, 2013, 1, 2354. | 2.7 | 27 |
| 400 | Torsional barriers of substituted biphenyls calculated using density functional theory: a benchmarking study. Organic and Biomolecular Chemistry, 2013, 11, 2859. | 1.5 | 51 |
| 401 | A Benchmark Study of H<sub>2</sub> Activation by Au<sub>3</sub> and Ag<sub>3</sub> Clusters. Journal of Physical Chemistry C, 2013, 117, 7487-7496. | 1.5 | 15 |
| 402 | Gas storage of simple molecules in boron oxide nanocapsules. International Journal of Quantum Chemistry, 2013, , n/a-n/a. | 1.0 | 1 |
| 403 | Perfluorophenylcalix[4]arenes: prospective hosts for nucleophilic guests. Synthesis, structure and quantum chemical calculations. Tetrahedron Letters, 2013, 54, 3496-3499. | 0.7 | 6 |
| 404 | The ammonium nitrate and its mechanism of decomposition in the gas phase: a theoretical study and a DFT benchmark. Physical Chemistry Chemical Physics, 2013, 15, 10849. | 1.3 | 43 |
| 405 | Theoretical Strategy to Build Structural Models of Microhydrated Inorganic Systems for the Knowledge of Their Vibrational Properties: The Case of the Hydrated Nitrate Aerosols. Journal of Physical Chemistry A, 2013, 117, 3826-3834. | 1.1 | 4 |
| 406 | Why is the reduction of NO in cytochrome c dependent nitric oxide reductase (cNOR) not electrogenic?. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 826-833. | 0.5 | 25 |
| 407 | Natures of benzene-water and pyrrole-water interactions in the forms of Ïƒ and Ï€ types: theoretical studies from clusters to liquid mixture. Journal of Molecular Modeling, 2013, 19, 1273-1283. | 0.8 | 17 |
| 408 | Mechanism and Selectivity of Bioinspired Cinchona Alkaloid Derivatives Catalyzed Asymmetric Olefin Isomerization: A Computational Study. Journal of the American Chemical Society, 2013, 135, 7462-7473. | 6.6 | 69 |
| 409 | Performance of dispersion-corrected double hybrid density functional theory: A computational study of OCS-hydrocarbon van der Waals complexes. Journal of Chemical Physics, 2013, 138, 164319. | 1.2 | 25 |
| 410 | 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. Journal of Chemical Theory and Computation, 2013, 9, 3240-3251. | 2.3 | 75 |
| 411 | Analytic derivatives for the XYG3 type of doubly hybrid density functionals: Theory, implementation, and assessment. Journal of Computational Chemistry, 2013, 34, 1759-1774. | 1.5 | 26 |
| 412 | Electronic Structure and Chemical Bonding in the OTiâ€“N<sub>2</sub> Complexes: A Systematic ab Initio and DFT Study. Journal of Physical Chemistry A, 2013, 117, 4462-4471. | 1.1 | 8 |
| 413 | Interplay between 1,3-Butadien-1,4-diyl and 2-Buten-1,4-dicarbene Derivatives: The Quest for Nucleophilic Carbenes. Journal of the American Chemical Society, 2013, 135, 8022-8030. | 6.6 | 18 |
| 414 | Strong lone pairâ‹¯Ï€ interactions between amine and tri-s-triazine derivatives: A theoretical investigation. Computational and Theoretical Chemistry, 2013, 1017, 144-152. | 1.1 | 7 |

| # | Article | IF | Citations |
|---|---|---|---|
| 415 | Is There Still Room for Parameter Free Double Hybrids? Performances of PBE0-DH and B2PLYP over Extended Benchmark Sets. Journal of Chemical Theory and Computation, 2013, 9, 3444-3452. | 2.3 | 37 |
| 416 | Improvement of Ïƒ1 receptor affinity by late-stage Câ€“H-bond arylation of spirocyclic lactones. Bioorganic and Medicinal Chemistry, 2013, 21, 1844-1856. | 1.4 | 98 |
| 417 | High-Level ab Initio Investigations on Structures and Energetics of N<sub>2</sub>O Clusters. Journal of Physical Chemistry A, 2013, 117, 8591-8598. | 1.1 | 10 |
| 418 | Aromatic Claisen Rearrangements of Oâ€Prenylated Tyrosine and Model Prenyl Aryl Ethers: Computational Study of the Role of Water on Acceleration of Claisen Rearrangements. European Journal of Organic Chemistry, 2013, 2013, 2823-2831. | 1.2 | 18 |
| 419 | Intermolecular interactions of formic acid with benzene: Energy decomposition analyses with ab initio MP2 and doubleâ€hybrid density functional computations. International Journal of Quantum Chemistry, 2013, 113, 2355-2360. | 1.0 | 12 |
| 420 | Which density functional is close to CCSD accuracy to describe geometry and interaction energy of small noncovalent dimers? A benchmark study using Gaussian09. Journal of Computational Chemistry, 2013, 34, 1341-1353. | 1.5 | 108 |
| 421 | Substrate Water Exchange for the Oxygen Evolving Complex in PSII in the S<sub>1</sub>, S<sub>2</sub>, and S<sub>3</sub> States. Journal of the American Chemical Society, 2013, 135, 9442-9449. | 6.6 | 102 |
| 422 | CH Stretching Region: Computational Modeling of Vibrational Optical Activity. Journal of Chemical Theory and Computation, 2013, 9, 3096-3108. | 2.3 | 29 |
| 423 | Methane CH Activation by Palladium Complexes with Chelating Bis(NHC) Ligands: A DFT Study. Organometallics, 2013, 32, 3469-3480. | 1.1 | 66 |
| 424 | Description of the Tautomerism in Some Azonaphthols. Journal of Physical Organic Chemistry, 2013, 26, 643-652. | 0.9 | 44 |
| 425 | Vibrational Spectra and Structures of Tiâ€“N<sub>2</sub>O and OTiâ€“N<sub>2</sub>: A Combined IR Matrix Isolation and Theoretical Study. Journal of Physical Chemistry A, 2013, 117, 1697-1705. | 1.1 | 5 |
| 426 | Quantum Monte Carlo Study of Ï€-Bonded Transition Metal Organometallics: Neutral and Cationic Vanadiumâ€“Benzene and Cobaltâ€“Benzene Half Sandwiches. Journal of Chemical Theory and Computation, 2013, 9, 390-400. | 2.3 | 21 |
| 427 | Dispersion corrected double high-hybrid and gradient-corrected density functional theory study of light cationâ€“dihydrogen (M+â€“H2, where MÂ=ÂLi, Na, B and Al) van der Waals complexes. Structural Chemistry, 2013, 24, 549-558. | 1.0 | 16 |
| 428 | Obtaining the lattice energy of the anthracene crystal by modern yet affordable first-principles methods. Journal of Chemical Physics, 2013, 138, 204304. | 1.2 | 17 |
| 429 | Binding in Radical-Solvent Binary Complexes: Benchmark Energies and Performance of Approximate Methods. Journal of Chemical Theory and Computation, 2013, 9, 1568-1579. | 2.3 | 46 |
| 430 | Reaching a Uniform Accuracy for Complex Molecular Systems: Long-Range-Corrected XYG3 Doubly Hybrid Density Functional. Journal of Physical Chemistry Letters, 2013, 4, 1669-1675. | 2.1 | 63 |
| 431 | Theoretical study of the photoelectron spectrum of ethyl formate: Ab initio and density functional theory investigation. European Physical Journal: Special Topics, 2013, 222, 2257-2266. | 1.2 | 8 |
| 432 | The Performance of Density Functionals for Sulfateâ€“Water Clusters. Journal of Chemical Theory and Computation, 2013, 9, 1368-1380. | 2.3 | 69 |

| # | Article | IF | Citations |
|---|---|---|---|
| 433 | Exploring Structures and Energetics of Large OCS Clusters by Correlated Methods. Journal of Physical Chemistry A, 2013, 117, 10964-10972. | 1.1 | 11 |
| 434 | Nonplanar Tertiary Amides in Rigid Chiral Tricyclic Dilactams. Peptide Group Distortions and Vibrational Optical Activity. Journal of Physical Chemistry B, 2013, 117, 9626-9642. | 1.2 | 7 |
| 435 | Polyoxometalate-Catalyzed Insertion of Oxygen from O2 into Tinâ€“Alkyl Bonds. Journal of the American Chemical Society, 2013, 135, 19304-19310. | 6.6 | 38 |
| 436 | Ramachandran Plot for Alanine Dipeptide as Determined from Raman Optical Activity. Journal of Physical Chemistry Letters, 2013, 4, 2763-2768. | 2.1 | 55 |
| 437 | A comparison of geometric parameters from PBE-based doubly hybrid density functionals PBE0-DH, PBE0-2, and xDH-PBE0. Journal of Chemical Physics, 2013, 139, 174106. | 1.2 | 32 |
| 438 | Theoretical investigation on the 2e/12c bond and second hyperpolarizability of azaphenalenyl radical dimers: Strength and effect of dimerization. Journal of Chemical Physics, 2013, 139, 124314. | 1.2 | 13 |
| 440 | How important is self-consistency for the dDsC density dependent dispersion correction?. Journal of Chemical Physics, 2014, 140, 18A516. | 1.2 | 24 |
| 442 | UV-tunable laser induced phototransformations of matrix isolated anethole. Journal of Chemical Physics, 2014, 140, 105102. | 1.2 | 6 |
| 443 | Systematic testing of Gaussian and complete basis set methods with dispersion corrections for environmentally relevant clusters. Chemical Physics Letters, 2014, 615, 50-55. | 1.2 | 1 |
| 444 | Kinetics of radicalâ€molecule reactions in aqueous solution: A benchmark study of the performance of density functional methods. Journal of Computational Chemistry, 2014, 35, 2019-2026. | 1.5 | 211 |
| 445 | Multiple Reaction Pathways Operating in the Mechanism of Vinylogous Mannichâ€Type Reaction Activated by a Water Molecule. Chemistry - an Asian Journal, 2014, 9, 305-312. | 1.7 | 12 |
| 446 | Accurate molecular structures and infrared spectra of trans-2,3-dideuterooxirane, methyloxirane, and trans-2,3-dimethyloxirane. Journal of Chemical Physics, 2014, 141, 034107. | 1.2 | 57 |
| 447 | Density Functional Theory Beyond the Generalized Gradient Approximation for Surface Chemistry. Topics in Current Chemistry, 2014, , 25-51. | 4.0 | 9 |
| 448 | Application of the Stabilized Koopmansâ€™ Theorem to the Temporary Anion States of Chlorosilanes in Longâ€Range Corrected Density Functional Theory. Journal of the Chinese Chemical Society, 2014, 61, 1313-1325. | 0.8 | 2 |
| 449 | A mechanophysical phase transition provides a dramatic example of colour polymorphism: the tribochromism of a substituted tri(methylene)tetrahydrofuran-2-one. Chemistry Central Journal, 2014, 8, 70. | 2.6 | 5 |
| 450 | Proton pumping in cytochrome c oxidase: Energetic requirements and the role of two proton channels. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, 1165-1177. | 0.5 | 38 |
| 451 | Halogen bonds with benzene: An assessment of DFT functionals. Journal of Computational Chemistry, 2014, 35, 386-394. | 1.5 | 73 |
| 452 | Photoinduced Excited State Electron Transfer at Liquid/Liquid Interfaces. Journal of Physical Chemistry B, 2014, 118, 7703-7714. | 1.2 | 9 |

| # | Article | IF | Citations |
|---|---|---|---|
| 453 | How Do DFT-DCP, DFT-NL, and DFT-D3 Compare for the Description of London-Dispersion Effects in Conformers and General Thermochemistry?. Journal of Chemical Theory and Computation, 2014, 10, 968-980. | 2.3 | 81 |
| 454 | Ions in solution: Density corrected density functional theory (DC-DFT). Journal of Chemical Physics, 2014, 140, 18A528. | 1.2 | 87 |
| 455 | Density Functional Theory in Quantum Chemistry. , 2014, , . | | 119 |
| 456 | Assessment of CCSD(T), MP2, DFT-D, CBS-QB3, and G4(MP2) methods for conformational study of alanine and proline dipeptides. Chemical Physics Letters, 2014, 600, 112-117. | 1.2 | 38 |
| 457 | Double-Hybrid Density Functionals Free of Dispersion and Counterpoise Corrections for Non-Covalent Interactions. Journal of Physical Chemistry A, 2014, 118, 3175-3182. | 1.1 | 23 |
| 458 | Structures and thermodynamic properties of (C2H6)n (n=2â€“8) by M06-2X and DFT-D theory: Implications for Titanâ€™s atmospheric chemistry. Chemical Physics Letters, 2014, 601, 194-199. | 1.2 | 1 |
| 459 | Construction of a parameter-free doubly hybrid density functional from adiabatic connection. Journal of Chemical Physics, 2014, 140, 18A512. | 1.2 | 57 |
| 461 | Anomeric effects in fluoro and trifluoromethyl piperidines: a computational study of conformational preferences and hydration. Theoretical Chemistry Accounts, 2014, 133, 1. | 0.5 | 5 |
| 462 | 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. Organometallics, 2014, 33, 847-857. | 1.1 | 43 |
| 463 | On the Innocence of Bipyridine Ligands: How Well Do DFT Functionals Fare for These Challenging Spin Systems?. Journal of Chemical Theory and Computation, 2014, 10, 220-235. | 2.3 | 34 |
| 464 | Stacking of the mutagenic DNA base analog 5-bromouracil. Theoretical Chemistry Accounts, 2014, 133, 1. | 0.5 | 9 |
| 465 | Fully anharmonic IR and Raman spectra of medium-size molecular systems: accuracy and interpretation. Physical Chemistry Chemical Physics, 2014, 16, 1759-1787. | 1.3 | 363 |
| 466 | Unraveling Organocuprate Complexity: Fundamental Insights into Intrinsic Group Transfer Selectivity in Alkylation Reactions. Journal of Organic Chemistry, 2014, 79, 1320-1334. | 1.7 | 21 |
| 467 | Quantum Chemical Studies of Mechanisms for Metalloenzymes. Chemical Reviews, 2014, 114, 3601-3658. | 23.0 | 494 |
| 468 | Computational modelling of oxygenation processes in enzymes and biomimetic model complexes. Chemical Communications, 2014, 50, 262-282. | 2.2 | 110 |
| 469 | A New-Generation Density Functional. Springer Briefs in Molecular Science, 2014, , . | 0.1 | 20 |
| 470 | Raman Spectroscopy of Conformational Rearrangements at Low Temperatures. Springer Theses, 2014, , . | 0.0 | 4 |
| 471 | Unbranched n-Alkanes. Springer Theses, 2014, , 37-117. | 0.0 | 2 |

| # | Article | IF | Citations |
|---|---|---|---|
| 472 | Addition of Câ€“C and Câ€“H bonds by pincer-iridium complexes: a combined experimental and computational study. Dalton Transactions, 2014, 43, 16354-16365. | 1.6 | 16 |
| 473 | Quantum-chemical insights into mixed-valence systems: within and beyond the Robinâ€“Day scheme. Chemical Society Reviews, 2014, 43, 5067-5088. | 18.7 | 168 |
| 474 | Quantum Chemical Investigations on Molecular Clusters. Chemical Reviews, 2014, 114, 12132-12173. | 23.0 | 170 |
| 475 | Benchmarking Calculated Lattice Parameters and Energies of Molecular Crystals Using van der Waals Density Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3423-3437. | 2.3 | 56 |
| 476 | Towards a quantitative understanding of palladium metal scavenger performance: an electronic structure calculation approach. Dalton Transactions, 2014, 43, 469-478. | 1.6 | 10 |
| 477 | Water oxidation energy diagrams for photosystem II for different protonation states, and the effect of removing calcium. Physical Chemistry Chemical Physics, 2014, 16, 11893. | 1.3 | 46 |
| 478 | Stretching and folding of 2-nanometer hydrocarbon rods. Soft Matter, 2014, 10, 4885-4901. | 1.2 | 28 |
| 479 | Non-radiative decay paths in rhodamines: new theoretical insights. Physical Chemistry Chemical Physics, 2014, 16, 20681-20688. | 1.3 | 44 |
| 480 | Theoretical study of efficiency of metal cations (Mg<sup>+</sup>, Ca<sup>+</sup>, and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 422 Td | 0.8 | 8 |
| 481 | Thermodynamic stability of PFOS: M06-2X and B3LYP comparison. Computational and Theoretical Chemistry, 2014, 1046, 81-92. | 1.1 | 22 |
| 482 | Atom Transfer Radical Polymerization (ATRP) and Organometallic Mediated Radical Polymerization (OMRP) of Styrene Mediated by Diaminobis(phenolato)iron(II) Complexes: A DFT Study. Inorganic Chemistry, 2014, 53, 7580-7590. | 1.9 | 40 |
| 483 | From Molecules to Materials: Computational Design of Nâ€Containing Porous Aromatic Frameworks for CO<sub>2</sub> Capture. ChemPhysChem, 2014, 15, 1772-1778. | 1.0 | 11 |
| 484 | Energy Diagrams for Water Oxidation in Photosystem II Using Different Density Functionals. Journal of Chemical Theory and Computation, 2014, 10, 268-272. | 2.3 | 47 |
| 485 | Some Observations on Counterpoise Corrections for Explicitly Correlated Calculations on Noncovalent Interactions. Journal of Chemical Theory and Computation, 2014, 10, 3791-3799. | 2.3 | 109 |
| 486 | Modeling of charge transfer processes to understand photophysical signatures: The case of Rhodamine 110. Chemical Physics Letters, 2014, 610-611, 148-152. | 1.2 | 17 |
| 487 | Benchmark Torsional Potentials of Building Blocks for Conjugated Materials: Bifuran, Bithiophene, and Biselenophene. Journal of Chemical Theory and Computation, 2014, 10, 3647-3655. | 2.3 | 41 |
| 488 | Investigating the Role of Solventâ€“Solute Interaction in Crystal Nucleation of Salicylic Acid from Organic Solvents. Journal of the American Chemical Society, 2014, 136, 11664-11673. | 6.6 | 98 |
| 489 | Doubleâ€hybrid density functionals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 576-600. | 6.2 | 292 |

| # | Article | IF | Citations |
|---|---|---|---|
| 490 | Intermolecular interactions in organic crystals: gaining insight from electronic structure analysis by density functional theory. CrystEngComm, 2014, 16, 7162-7171. | 1.3 | 10 |
| 491 | van der <scp>W</scp>aals corrected density functional calculations of the adsorption of benzene on the Cu (111) surface. Journal of Computational Chemistry, 2014, 35, 2263-2271. | 1.5 | 11 |
| 492 | Chlorination of N-Methylacetamide and Amide-Containing Pharmaceuticals. Quantum-Chemical Study of the Reaction Mechanism. Journal of Physical Chemistry A, 2014, 118, 2367-2376. | 1.1 | 20 |
| 493 | Influence of Solvent and Solid-State Structure on Nucleation of Parabens. Crystal Growth and Design, 2014, 14, 3890-3902. | 1.4 | 54 |
| 494 | Coordination of Halide and Chalcogenolate Anions to Heavier 1,2,5-Chalcogenadiazoles: Experiment and Theory. Organometallics, 2014, 33, 4302-4314. | 1.1 | 60 |
| 495 | Fractional Charge Behavior and Band Gap Predictions with the XYG3 Type of Doubly Hybrid Density Functionals. Journal of Physical Chemistry A, 2014, 118, 9201-9211. | 1.1 | 45 |
| 496 | Direct observation of two-electron Ag(I)/Ag(III) redox cycles in coupling catalysis. Nature Communications, 2014, 5, 4373. | 5.8 | 65 |
| 497 | Theoretical Study of the Water Oxidation Mechanism with Non-heme Fe(Pytacn) Iron Complexes. Evidence That the Fe<sup>IV</sup>(O)(Pytacn) Species Cannot React with the Water Molecule To Form the Oâ€“O Bond. Inorganic Chemistry, 2014, 53, 5474-5485. | 1.9 | 40 |
| 498 | Assessment of dispersionâ€improved exchangeâ€correlation functionals for the simulation of CO<sub>2</sub> binding by alcoholamines. International Journal of Quantum Chemistry, 2014, 114, 805-812. | 1.0 | 14 |
| 499 | Unraveling the Mechanism of Water Oxidation Catalyzed by Nonheme Iron Complexes. Chemistry - A European Journal, 2014, 20, 5696-5707. | 1.7 | 75 |
| 500 | Density functional theory: Foundations reviewed. Physics Reports, 2014, 544, 123-239. | 10.3 | 91 |
| 501 | Bâ€“H Bond Cleavage via Metalâ€“Ligand Cooperation by Dearomatized Ruthenium Pincer Complexes. Organometallics, 2014, 33, 3716-3726. | 1.1 | 48 |
| 502 | Stable Saltâ€“Water Cluster Structures Reflect the Delicate Competition between Ionâ€“Water and Waterâ€“Water Interactions. Journal of Physical Chemistry B, 2014, 118, 743-751. | 1.2 | 39 |
| 503 | Conformational Properties of Oxazole-Amino Acids: Effect of the Intramolecular Nâ€“HÂ·Â·Â·N Hydrogen Bond. Journal of Physical Chemistry B, 2014, 118, 2340-2350. | 1.2 | 17 |
| 504 | Determination of the Absolute Configuration of Perylene Quinoneâ€Derived Mycotoxins by Measurement and Calculation of Electronic Circular Dichroism Spectra and Specific Rotations. Chemistry - A European Journal, 2014, 20, 11463-11470. | 1.7 | 24 |
| 505 | Performance of DFT methods and origin of stereoselectivity in bipyridine N,Nâ€²-dioxide catalyzed allylation and propargylation reactions. Organic and Biomolecular Chemistry, 2014, 12, 8346-8353. | 1.5 | 18 |
| 506 | An Angular Overlap Model for Cu(II) Ion in the AMOEBA Polarizable Force Field. Journal of Chemical Theory and Computation, 2014, 10, 298-311. | 2.3 | 28 |
| 507 | Stacking interactions of nickel bis(dithiolene) with benzene. Chemical Physics Letters, 2014, 591, 29-31. | 1.2 | 1 |

| # | Article | IF | Citations |
|---|---|---|---|
| 508 | Molecular Structure and Spectroscopic Signatures of Acrolein: Theory Meets Experiment. Journal of Physical Chemistry A, 2014, 118, 6648-6656. | 1.1 | 37 |
| 509 | Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection. Journal of Chemical Theory and Computation, 2014, 10, 3074-3084. | 2.3 | 161 |
| 510 | Role of the Isolable Hydride Intermediate in the Hydrosilylation of Carbonyl Compounds Catalyzed by the Highâ€Valent Monoâ€Oxidoâ€“Rhenium(V) Complex. European Journal of Inorganic Chemistry, 2014, 2014, 5714-5723. | 1.0 | 9 |
| 511 | A Mechanistic Study of the Spontaneous Hydrolysis of Glycylserine as the Simplest Model for Protein Selfâ€Cleavage. Chemistry - A European Journal, 2014, 20, 456-466. | 1.7 | 17 |
| 512 | Quantum-mechanical study of energies, structures, and vibrational spectra of the H(D)Cl complexed with dimethyl ether. Journal of Chemical Physics, 2015, 143, 204302. | 1.2 | 2 |
| 513 | Thermodynamic stability of neutral and anionic PFOAs. Theoretical Chemistry Accounts, 2015, 134, 1. | 0.5 | 6 |
| 514 | Mechanistic Aspects of Arylâ€“Halide Oxidative Addition, Coordination Chemistry, and Ringâ€Walking by Palladium. Chemistry - A European Journal, 2015, 21, 16113-16125. | 1.7 | 11 |
| 515 | Water Oxidation for Simplified Models of the Oxygenâ€Evolving Complex in Photosystemâ€…II. Chemistry - A European Journal, 2015, 21, 18821-18827. | 1.7 | 11 |
| 516 | Going clean: structure and dynamics of peptides in the gas phase and paths to solvation. Journal of Physics Condensed Matter, 2015, 27, 493002. | 0.7 | 29 |
| 517 | Critical evaluation of the potential energy surface of the CH3 + HO2reaction system. Journal of Chemical Physics, 2015, 142, 054308. | 1.2 | 11 |
| 518 | Global Hybrids from the Semiclassical Atom Theory Satisfying the Local Density Linear Response. Journal of Chemical Theory and Computation, 2015, 11, 122-131. | 2.3 | 22 |
| 519 | A theoretical study on mitigation of CO2 through advanced deep eutectic solvents. International Journal of Greenhouse Gas Control, 2015, 39, 62-73. | 2.3 | 55 |
| 520 | Revisiting the Passerini Reaction Mechanism: Existence of the Nitrilium, Organocatalysis of Its Formation, and Solvent Effect. Journal of Organic Chemistry, 2015, 80, 5652-5657. | 1.7 | 62 |
| 521 | Inquiry of the reaction paths in thermal retro-Dielsâ€“Alder reactions in the gas phase: Theoretical study on the concerted and stepwise elimination mechanisms of cyclohexenes. Computational and Theoretical Chemistry, 2015, 1067, 103-113. | 1.1 | 3 |
| 522 | Reaction Network of Methanol Synthesis over Cu/ZnO Nanocatalysts. ACS Catalysis, 2015, 5, 4201-4218. | 5.5 | 87 |
| 523 | Interaction between PH3 and small water clusters: Understanding the electronic and spectroscopic properties. Computational and Theoretical Chemistry, 2015, 1059, 35-44. | 1.1 | 21 |
| 524 | Benchmarking Ground-State Geometries and Vertical Excitation Energies of a Selection of P-Type Semiconducting Molecules with Different Polarity. Journal of Physical Chemistry A, 2015, 119, 12876-12891. | 1.1 | 25 |
| 525 | Noncovalent Interactions of Heteroboranes. Challenges and Advances in Computational Chemistry and Physics, 2015, , 219-239. | 0.6 | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 526 | Interplay of experiment and theory: high resolution infrared spectrum and accurate equilibrium structure of BF<sub>2</sub>OH. Physical Chemistry Chemical Physics, 2015, 17, 30440-30449. | 1.3 | 18 |
| 528 | Energy dissipative photoprotective mechanism of carotenoid spheroidene from the photoreaction center of purple bacteria Rhodobacter sphaeroides. Physical Chemistry Chemical Physics, 2015, 17, 23468-23480. | 1.3 | 4 |
| 529 | NTChem: A highâ€performance software package for quantum molecular simulation. International Journal of Quantum Chemistry, 2015, 115, 349-359. | 1.0 | 55 |
| 530 | Mechanistic Investigation Into Catalytic Hydrosilylation with a High-Valent Ruthenium(VI)â€“Nitrido Complex: A DFT Study. Organometallics, 2015, 34, 212-220. | 1.1 | 13 |
| 531 | Benchmark of electronic structure methods for proteinâ€“ligand interactions based on high-level reference data. Journal of Theoretical and Computational Chemistry, 2015, 14, 1540001. | 1.8 | 7 |
| 532 | A computational study on high-valent mono-oxo-rhenium(V) complex-catalyzed hydrosilylation of carbonyls: What a difference an oxo ligand makes. Journal of Molecular Catalysis A, 2015, 400, 31-41. | 4.8 | 7 |
| 533 | Density Functional Theory and Hydrogen Bonds: Are We There Yet?. ChemPhysChem, 2015, 16, 978-985. | 1.0 | 129 |
| 534 | Error Accumulations in Adhesive Energies of Dihydrogen Molecular Chains: Performances of the XYG3 Type of Doubly Hybrid Density Functionals. Journal of Physical Chemistry A, 2015, 119, 1590-1599. | 1.1 | 13 |
| 535 | Dispersion Interactions between Urea and Nucleobases Contribute to the Destabilization of RNA by Urea in Aqueous Solution. Journal of Physical Chemistry B, 2015, 119, 3755-3761. | 1.2 | 16 |
| 536 | Microsolvation of 2-Thiouracil: Molecular Structure and Spectroscopic Parameters of the Thiouracilâ€“Water Complex. Journal of Physical Chemistry A, 2015, 119, 5386-5395. | 1.1 | 22 |
| 537 | Exploring the Aqueous Vertical Ionization of Organic Molecules by Molecular Simulation and Liquid Microjet Photoelectron Spectroscopy. Journal of Physical Chemistry B, 2015, 119, 238-256. | 1.2 | 32 |
| 538 | Dimerization of Two Alkyne Units: Model Studies, Intermediate Trapping Experiments, and Kinetic Studies. Journal of the American Chemical Society, 2015, 137, 1833-1843. | 6.6 | 41 |
| 539 | Physical and Thermodynamic Properties of Al<sub>n</sub>C<sub>m</sub> Clusters: Quantum-Chemical Study. Journal of Physical Chemistry A, 2015, 119, 1369-1380. | 1.1 | 29 |
| 540 | Direct and Indirect Effects of Dispersion Interactions on the Electric Properties of Weakly Bound Complexes. Journal of Physical Chemistry A, 2015, 119, 3112-3124. | 1.1 | 12 |
| 541 | The role of density functional theory methods in the prediction of nanostructured gas-adsorbent materials. Coordination Chemistry Reviews, 2015, 300, 142-163. | 9.5 | 36 |
| 542 | Encapsulated Guests in the Smallest Spaces: Shrinking Guests by Compression and Investigations under Solvent-Free Conditions. Journal of Organic Chemistry, 2015, 80, 8065-8072. | 1.7 | 5 |
| 543 | First-Principles Predictions of Vibrational Raman Optical Activity of Globular Proteins. Journal of Physical Chemistry Letters, 2015, 6, 3314-3319. | 2.1 | 56 |
| 544 | A detailed study of cholinium chloride and levulinic acid deep eutectic solvent system for CO<sub>2</sub> capture via experimental and molecular simulation approaches. Physical Chemistry Chemical Physics, 2015, 17, 20941-20960. | 1.3 | 133 |

| # | Article | IF | Citations |
|---|---|---|---|
| 545 | Molecular hydrogen binding affinities of metal cation decorated substituted benzene systems: insight from computational exploration. RSC Advances, 2015, 5, 57647-57656. | 1.7 | 8 |
| 546 | Theoretical Study on the Solvation of C<sub>60</sub> Fullerene by Ionic Liquids II: DFT Analysis of the Interaction Mechanism. Journal of Physical Chemistry B, 2015, 119, 10616-10629. | 1.2 | 9 |
| 547 | An approach for the rationalization of melting temperature for deep eutectic solvents from DFT. Chemical Physics Letters, 2015, 634, 151-155. | 1.2 | 111 |
| 548 | Enediyne Dimerization vs Bergman Cyclization. Organic Letters, 2015, 17, 1425-1428. | 2.4 | 18 |
| 549 | Water Effect on Acid-Gas Capture Using Choline Lactate: A DFT Insight beyond Moleculeâ€“Molecule Pair Simulations. Journal of Physical Chemistry B, 2015, 119, 5546-5557. | 1.2 | 14 |
| 550 | A density functional theory insight towards the rational design of ionic liquids for SO<sub>2</sub> capture. Physical Chemistry Chemical Physics, 2015, 17, 13559-13574. | 1.3 | 37 |
| 551 | Theoretical Study of the Reactions of Ethanol with Aluminum and Aluminum Oxide. Journal of Physical Chemistry A, 2015, 119, 3897-3904. | 1.1 | 15 |
| 552 | The Unexpected Mechanism Underlying the Highâ€Valent Monoâ€Oxoâ€Rhenium(V) Hydride Catalyzed Hydrosilylation of Cï£¾N Functionalities: Insights from a DFT Study. ChemPhysChem, 2015, 16, 1052-1060. | 1.0 | 5 |
| 553 | From Thermodynamics to Kinetics: Enhanced Sampling of Rare Events. Accounts of Chemical Research, 2015, 48, 947-955. | 7.6 | 66 |
| 554 | Alternative mechanisms for O<sub>2</sub>release and Oâ€“O bond formation in the oxygen evolving complex of photosystem II. Physical Chemistry Chemical Physics, 2015, 17, 12168-12174. | 1.3 | 97 |
| 555 | Model Studies on the Dimerization of 1,3-Diacetylenes. Journal of Organic Chemistry, 2015, 80, 5077-5083. | 1.7 | 11 |
| 556 | Explicit solvent simulations of the aqueous oxidation potential and reorganization energy for neutral molecules: gas phase, linear solvent response, and non-linear response contributions. Physical Chemistry Chemical Physics, 2015, 17, 14811-14826. | 1.3 | 19 |
| 557 | Influence of Microstructure and Interaction on Viscosity of Ionic Liquids. Industrial & Engineering Chemistry Research, 2015, 54, 3505-3514. | 1.8 | 51 |
| 558 | Steering Power of Perfluoroalkyl Substituents in Crystal Engineering: Tuning the Ï€â€“Ï€ Distance While Maintaining the Lamellar Packing Motif for Aromatics with Various Sizes of Ï€-Conjugation. Crystal Growth and Design, 2015, 15, 2235-2242. | 1.4 | 17 |
| 559 | Molecular Mechanism of NDMA Formation from N,N-Dimethylsulfamide During Ozonation: Quantum Chemical Insights into a Bromide-Catalyzed Pathway. Environmental Science & Technology, 2015, 49, 4163-4175. | 4.6 | 53 |
| 560 | Density Functional Theory Study on the Cholinium Dihydrogenphosphate Ionic Liquid for Acid Gas Removal. Journal of Solution Chemistry, 2015, 44, 890-899. | 0.6 | 3 |
| 561 | Benchmark thermochemistry of chloramines, bromamines, and bromochloramines: halogen oxidants stabilized by electron correlation. Physical Chemistry Chemical Physics, 2015, 17, 3584-3598. | 1.3 | 8 |
| 562 | Quantum Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins. Journal of Chemical Theory and Computation, 2015, 11, 4992-5001. | 2.3 | 42 |

| # | Article | IF | Citations |
|---|---|---|---|
| 563 | Electromers of the benzene dimer radical cation. Physical Chemistry Chemical Physics, 2015, 17, 10624-10629. | 1.3 | 8 |
| 564 | Understanding the Boronâ€“Nitrogen Interaction and Its Possible Implications in Drug Design. Journal of Physical Chemistry B, 2015, 119, 14393-14401. | 1.2 | 5 |
| 565 | A computational study of the chlorination and hydroxylation of amines by hypochlorous acid. Organic and Biomolecular Chemistry, 2015, 13, 11740-11752. | 1.5 | 23 |
| 566 | CC/DFT Route toward Accurate Structures and Spectroscopic Features for Observed and Elusive Conformers of Flexible Molecules: Pyruvic Acid as a Case Study. Journal of Chemical Theory and Computation, 2015, 11, 4342-4363. | 2.3 | 75 |
| 567 | Stereoelectronic source of the anomalous stability of bis-peroxides. Chemical Science, 2015, 6, 6783-6791. | 3.7 | 79 |
| 568 | Assessment of DFT methods for studying acid gas capture by ionic liquids. Physical Chemistry Chemical Physics, 2015, 17, 26875-26891. | 1.3 | 27 |
| 569 | Quantum Chemical Benchmark Study on 46 RNA Backbone Families Using a Dinucleotide Unit. Journal of Chemical Theory and Computation, 2015, 11, 4972-4991. | 2.3 | 90 |
| 570 | Ferricâ€“Thiolate Bond Dissociation Studied with Electronic Structure Calculations. Journal of Physical Chemistry A, 2015, 119, 10084-10090. | 1.1 | 12 |
| 571 | anti-Diradical Formation in 1,3-Dipolar Cycloadditions of Nitrile Oxides to Acetylenes. Journal of Organic Chemistry, 2015, 80, 12321-12332. | 1.7 | 29 |
| 572 | Rhodium catalysed conversion of carbenes into ketenes and ketene imines using PNN pincer complexes. Organic Chemistry Frontiers, 2015, 2, 1561-1577. | 2.3 | 31 |
| 573 | Local response dispersion method: A densityâ€dependent dispersion correction for density functional theory. International Journal of Quantum Chemistry, 2015, 115, 309-324. | 1.0 | 12 |
| 574 | Non-parametrized functionals with empirical dispersion corrections: A happy match?. Theoretical Chemistry Accounts, 2015, 134, 1. | 0.5 | 16 |
| 575 | Analytical Double-Hybrid Density Functional Based on the Polynomial Series Expansion of Adiabatic Connection: A Quadratic Approximation. Journal of Chemical Theory and Computation, 2015, 11, 45-54. | 2.3 | 22 |
| 576 | Hydrogen-bonding interactions between a pyridinium-based ionic liquid [C4Py][SCN] and dimethyl sulfoxide. Chemical Engineering Science, 2015, 121, 169-179. | 1.9 | 40 |
| 577 | Spectroscopic and ab initio investigation of 2,6-difluorophenylacetyleneâ€“amine complexes: coexistence of Câ€“Hâ‹¯N and lone-pairâ‹¯Ï€ complexes and intermolecular coulombic decay. Physical Chemistry Chemical Physics, 2015, 17, 434-443. | 1.3 | 14 |
| 578 | Computational study of unsaturated and saturated cyclic (alkyl) (amino) carbene borane complexes. Computational and Theoretical Chemistry, 2015, 1051, 17-23. | 1.1 | 3 |
| 579 | 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. Organic and Biomolecular Chemistry, 2015, 13, 807-816. | 1.5 | 7 |
| 580 | Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215. | 0.8 | 2,561 |

| # | Article | IF | Citations |
|---|---|---|---|
| 581 | Assessment of Contemporary Theoretical Methods for Bond Dissociation Enthalpies. Chinese Journal of Chemical Physics, 2016, 29, 453-461. | 0.6 | 6 |
| 582 | Nonoxido V<sup>IV</sup> Complexes: Prediction of the EPR Spectrum and Electronic Structure of Simple Coordination Compounds and Amavadin. Inorganic Chemistry, 2016, 55, 7373-7387. | 1.9 | 35 |
| 583 | Comparison of oneâ€parameter and linearly scaled oneâ€parameter doubleâ€hybrid density functionals for noncovalent interactions. International Journal of Quantum Chemistry, 2016, 116, 1166-1172. | 1.0 | 5 |
| 584 | Geometries and properties of the heterobimetallic phosphido-bridged complex:. Journal of Structural Chemistry, 2016, 57, 1019-1023. | 0.3 | 1 |
| 585 | Vibrational infrared and Raman spectra of polypeptides: Fragments-in-fragments within molecular tailoring approach. Journal of Chemical Physics, 2016, 144, 114113. | 1.2 | 32 |
| 586 | Advanced catalyst design induced enhancement of multi-walled nanotube debundling and electrical conductivity of multi-walled nanotube/silicone composites. RSC Advances, 2016, 6, 48120-48128. | 1.7 | 4 |
| 587 | Ability of density functional theory methods to accurately model the reaction energy pathways of the oxidation of CO on gold cluster: A benchmark study. Theoretical Chemistry Accounts, 2016, 135, 1. | 0.5 | 11 |
| 588 | Recent development of atomâ€pairwise van der waals corrections for density functional theory: From molecules to solids. International Journal of Quantum Chemistry, 2016, 116, 598-607. | 1.0 | 19 |
| 589 | Troubles in the Systematic Prediction of Transition Metal Thermochemistry with Contemporary Out-of-the-Box Methods. Journal of Chemical Theory and Computation, 2016, 12, 1542-1560. | 2.3 | 42 |
| 590 | Hydrogen transfer between dimethyl ether and the methoxy radical: Understanding and kinetic modeling with anharmonic torsions. Computational and Theoretical Chemistry, 2016, 1089, 43-53. | 1.1 | 6 |
| 591 | A spectroscopic and theoretical study in the near-infrared region of low concentration aliphatic alcohols. Physical Chemistry Chemical Physics, 2016, 18, 13666-13682. | 1.3 | 72 |
| 592 | Origin of the Catalytic Effects of Molecular Iodine: A Computational Analysis. ACS Catalysis, 2016, 6, 3203-3212. | 5.5 | 108 |
| 593 | Dispersion-Corrected Mean-Field Electronic Structure Methods. Chemical Reviews, 2016, 116, 5105-5154. | 23.0 | 1,032 |
| 594 | Comprehensive Energetic Scale for Quantitatively Estimating the Fluorinating Potential of Nâ€“F Reagents in Electrophilic Fluorinations. Journal of Organic Chemistry, 2016, 81, 4280-4289. | 1.7 | 50 |
| 595 | The nature of inter- and intramolecular interactions in F2OXeâ¦HX (X= F, Cl, Br, I) complexes. Journal of Molecular Modeling, 2016, 22, 119. | 0.8 | 1 |
| 596 | Beyond energies: geometry predictions with the XYG3 type of doubly hybrid density functionals. Chemical Communications, 2016, 52, 13840-13860. | 2.2 | 18 |
| 597 | Understanding and modeling the hydrogen-abstraction from dimethyl ether by the methyl radical with torsional anharmonicity. Computational and Theoretical Chemistry, 2016, 1096, 7-16. | 1.1 | 3 |
| 598 | Dehydrogenation of benzyl alcohol with N<sub>2</sub>O as the hydrogen acceptor catalyzed by the rhodium(<scp>i</scp>) carbene complex: insights from quantum chemistry calculations. Dalton Transactions, 2016, 45, 16485-16491. | 1.6 | 10 |

| # | Article | IF | Citations |
|---|---|---|---|
| 599 | The 1,2-hydrogen shift reaction for monohalogenophosphanes PH<sub>2</sub>X and HPX (XÂ= F, Cl). Molecular Physics, 2016, 114, 2999-3014. | 0.8 | 3 |
| 600 | Failure of Density Functional Dispersion Correction in Metallic Systems and Its Possible Solution Using a Modified Many-Body Dispersion Correction. Journal of Physical Chemistry Letters, 2016, 7, 3278-3283. | 2.1 | 13 |
| 601 | The INV24 test set: how well do quantum-chemical methods describe inversion and racemization barriers?. Canadian Journal of Chemistry, 2016, 94, 1133-1143. | 0.6 | 45 |
| 602 | Model Calculations Suggest that the Central Carbon in the FeMo-Cofactor of Nitrogenase Becomes Protonated in the Process of Nitrogen Fixation. Journal of the American Chemical Society, 2016, 138, 10485-10495. | 6.6 | 92 |
| 603 | Assessing One- and Two-Photon Optical Properties of Boron Containing Arenes. Journal of Physical Chemistry C, 2016, 120, 17916-17926. | 1.5 | 30 |
| 604 | Explicit Polarization Theory. , 2016, , 51-82. | | 2 |
| 605 | A unified set of experimental organometallic data used to evaluate modern theoretical methods. Dalton Transactions, 2016, 45, 13766-13778. | 1.6 | 24 |
| 606 | 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 |
| 607 | [Al<sub>2</sub>O<sub>4</sub>]<sup>â^'</sup>, a Benchmark Gas-Phase Class II Mixed-Valence Radical Anion for the Evaluation of Quantum-Chemical Methods. Journal of Chemical Theory and Computation, 2016, 12, 3796-3806. | 2.3 | 20 |
| 608 | New progress in theoretical studies on palladium-catalyzed Câ^'C bond-forming reaction mechanisms. Science China Chemistry, 2016, 59, 1432-1447. | 4.2 | 24 |
| 609 | Aiming at an accurate prediction of vibrational and electronic spectra for mediumâ€toâ€large molecules: An overview. International Journal of Quantum Chemistry, 2016, 116, 1543-1574. | 1.0 | 161 |
| 610 | Assessment of DFT Functionals for QTAIM Topological Analysis of Halogen Bonds with Benzene. Journal of Physical Chemistry A, 2016, 120, 9071-9080. | 1.1 | 37 |
| 611 | Prediction of heat of formation for exo -Dicyclopentadiene. Journal of Loss Prevention in the Process Industries, 2016, 44, 433-439. | 1.7 | 7 |
| 612 | Insights into choline chlorideâ€“phenylacetic acid deep eutectic solvent for CO<sub>2</sub> absorption. RSC Advances, 2016, 6, 109201-109210. | 1.7 | 31 |
| 613 | Investigations on isolated peptides by combined IR/UV spectroscopy in a molecular beam â€“ structure, aggregation, solvation and molecular recognition. International Reviews in Physical Chemistry, 2016, 35, 569-677. | 0.9 | 51 |
| 614 | A quantum chemical study of HOCl-induced transformations of carbamazepine. Organic and Biomolecular Chemistry, 2016, 14, 10866-10874. | 1.5 | 11 |
| 615 | Investigation into the Solid and Solution Properties of Known and Novel Polymorphs of the Antimicrobial Molecule Clofazimine. Crystal Growth and Design, 2016, 16, 7240-7250. | 1.4 | 21 |
| 616 | Thermochemistry and Geometries for Transition-Metal Chemistry from the Random Phase Approximation. Journal of Chemical Theory and Computation, 2016, 12, 5350-5360. | 2.3 | 21 |

| # | Article | IF | Citations |
|---|---|---|---|
| 617 | Van der Waals interactions and the limits of isolated atom models at interfaces. Nature Communications, 2016, 7, 11559. | 5.8 | 111 |
| 618 | Influence of mutations at the proximal histidine position on the Feâ€“O2 bond in hemoglobin from density functional theory. Journal of Chemical Physics, 2016, 144, 095101. | 1.2 | 2 |
| 619 | Substituent effects on gasâ€phase homolytic Feâ€“O and Feâ€“S bond energies of mâ€Câ€<sub>6</sub>H<sub>4</sub>OFe(CO)<sub>2</sub>(Î·<sup>5</sup>â€C<sub>5</sub>H<sub>5</sub>) and mâ€Câ€<sub>6</sub>H<sub>4</sub>SFe(CO)<sub>2</sub>(Î·<sup>5</sup>â€C<sub>5</sub>H<sub>5</sub>) studied using Hartreeâ€“Fock and density functional theory methods. Journal of Physical Organic Chemistry, 2016, 29, 172-184. | 0.9 | 5 |
| 620 | New Insights into Mechanism of Molybdenum(VI)â€“Dioxo Complex Catalyzed Hydrosilylation of Carbonyls: An Alternative Model for Activating Siâ€“H Bond. Journal of Physical Chemistry A, 2016, 120, 4167-4178. | 1.1 | 6 |
| 621 | On the inclusion of postâ€<scp>MP</scp>2 contributions to doubleâ€Hybrid density functionals. Journal of Computational Chemistry, 2016, 37, 183-193. | 1.5 | 30 |
| 622 | Conformational preferences and synthesis of isomers Z and E of oxazoleâ€dehydrophenylalanine. Biopolymers, 2016, 106, 283-294. | 1.2 | 5 |
| 623 | Gas phase enthalpies of formation, isomerization, and disproportionation of mono- through tetra-substituted tetrahedranes: A G4(MP2)/G4 theoretical study. Computational and Theoretical Chemistry, 2016, 1075, 30-37. | 1.1 | 5 |
| 624 | Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks for Ground-State Properties. Journal of Chemical Theory and Computation, 2016, 12, 1097-1120. | 2.3 | 74 |
| 625 | N-heterocyclic carbene-stabilized homoatomic lithium(0) complexes with a lithiumâ€“lithium covalent bond: A theoretical design and characterization. Inorganic Chemistry Communication, 2016, 63, 61-64. | 1.8 | 3 |
| 626 | Computational methods for the description of pharmacologically relevant platinum complexes â€“ molecular structure and bond dissociation. Physical Chemistry Chemical Physics, 2016, 18, 4051-4062. | 1.3 | 4 |
| 627 | Interaction mechanism of doxorubicin and SWCNT: protonation and diameter effects on drug loading and releasing. RSC Advances, 2016, 6, 314-322. | 1.7 | 63 |
| 628 | Electron Detachment and Subsequent Structural Changes of Water Clusters. Journal of Physical Chemistry A, 2016, 120, 1065-1073. | 1.1 | 5 |
| 629 | Reliable vibrational wavenumbers for Cî€O and Nâ€“H stretchings of isolated and hydrogen-bonded nucleic acid bases. Physical Chemistry Chemical Physics, 2016, 18, 8479-8490. | 1.3 | 47 |
| 630 | Simulations of Gas Adsorption in Thiophene-Based Cyclo-1,4-phenylene-2â€²,5â€²-thienylenes Using First-Principles-derived Force Field. Journal of Physical Chemistry C, 2016, 120, 4329-4336. | 1.5 | 2 |
| 631 | Coordination and insertion of alkenes and alkynes in Au<sup>III</sup>complexes: nature of the intermediates from a computational perspective. Dalton Transactions, 2016, 45, 5504-5513. | 1.6 | 20 |
| 632 | Interactions between metal cations with H2 in the M+- H2 complexes: Performance of DFT and DFT-D methods. Journal of Chemical Sciences, 2016, 128, 621-631. | 0.7 | 16 |
| 633 | The S66x8 benchmark for noncovalent interactions revisited: explicitly correlated ab initio methods and density functional theory. Physical Chemistry Chemical Physics, 2016, 18, 20905-20925. | 1.3 | 182 |
| 634 | Reactions of Chemically Activated Formic Acid Formed via HÄŠO + È®H. Journal of Physical Chemistry A, 2016, 120, 1819-1824. | 1.1 | 9 |

| # | Article | IF | Citations |
|---|---|---|---|
| 635 | Benchmark ab Initio Conformational Energies for the Proteinogenic Amino Acids through Explicitly Correlated Methods. Assessment of Density Functional Methods. Journal of Chemical Theory and Computation, 2016, 12, 444-454. | 2.3 | 99 |
| 636 | Benchmarking semiempirical, Hartreeâ€“Fock, DFT, and MP2 methods against the ionization energies and electron affinities of short- through long-chain [n]acenes and [n]phenacenes. Canadian Journal of Chemistry, 2016, 94, 251-258. | 0.6 | 8 |
| 637 | Quantum chemical study of the reactions of Al, AlO and AlOH with H2O2. Chemical Physics, 2016, 465-466, 9-16. | 0.9 | 6 |
| 638 | Theoretical study on fluorescent probes for cyanide based on the indolium functional group. Organic Electronics, 2016, 30, 1-11. | 1.4 | 8 |
| 639 | Buckminster fullerene adhesion on graphene flakes: Numerical accuracy of dispersion corrected DFT. Polyhedron, 2016, 114, 110-117. | 1.0 | 8 |
| 640 | Modelling of graphene functionalization. Physical Chemistry Chemical Physics, 2016, 18, 6351-6372. | 1.3 | 190 |
| 641 | Density functional theory study of substituent effects on gasâ€phase heterolytic Feâ€“O and Feâ€“S bond energies of mâ€Câ€<sub>6</sub>H<sub>4</sub>OFe(CO)<sub>2</sub>(Î·<sup>5</sup>â€C<sub>5</sub>H<sub>5</sub>) and mâ€Câ€<sub>6</sub>H<sub>4</sub>SFe(CO)<sub>2</sub>(Î·<sup>5</sup>â€C<sub>5</sub>H<sub>5</sub>). Journal of Physical Organic Chemistry, 2017, 30, e3582. | 0.9 | 3 |
| 642 | Efficient algorithm for multiconfiguration pair-density functional theory with application to the heterolytic dissociation energy of ferrocene. Journal of Chemical Physics, 2017, 146, 034101. | 1.2 | 29 |
| 643 | Computational Studies on Reaction Mechanism and Origins of Selectivities in Nickel-Catalyzed (2 + 2 +) Tj ETQq0 0 0 rgBT /Overlock 10 Chemistry, 2017, 82, 2150-2159. | 1.7 | 10 |
| 644 | Long-range interactions from the many-pair expansion: A different avenue to dispersion in DFT. Journal of Chemical Physics, 2017, 146, 024111. | 1.2 | 6 |
| 645 | Building block candidates for the design of proton exchange membranes: Maleimide and its homologues. International Journal of Hydrogen Energy, 2017, 42, 515-526. | 3.8 | 0 |
| 646 | Quantum Chemical Methods for the Prediction of Energetic, Physical, and Spectroscopic Properties of Ionic Liquids. Chemical Reviews, 2017, 117, 6696-6754. | 23.0 | 181 |
| 647 | Understanding the role of Zn<sup>2+</sup> in the hydrolysis of glycylserine: a mechanistic study by using density functional theory. Molecular Physics, 2017, 115, 403-412. | 0.8 | 3 |
| 648 | The Effect of Conjugation on the Competition between Internal Conversion and Electron Detachment: A Comparison between Green Fluorescent and Red Kaede Protein Chromophores. Journal of Physical Chemistry Letters, 2017, 8, 765-771. | 2.1 | 17 |
| 649 | Variational Effect and Anharmonic Torsion on Kinetic Modeling for Initiation Reaction of Dimethyl Ether Combustion. Journal of Physical Chemistry A, 2017, 121, 1121-1132. | 1.1 | 12 |
| 650 | Empirical D3 Dispersion as a Replacement for ab Initio Dispersion Terms in Density Functional Theory-Based Symmetry-Adapted Perturbation Theory. Journal of Chemical Theory and Computation, 2017, 13, 1638-1646. | 2.3 | 11 |
| 651 | Mechanism of extractive/oxidative desulfurization using the ionic liquid inimidazole acetate: a computational study. Journal of Molecular Modeling, 2017, 23, 54. | 0.8 | 4 |
| 652 | Partnering dispersion corrections with modern parameter-free double-hybrid density functionals. Physical Chemistry Chemical Physics, 2017, 19, 13481-13487. | 1.3 | 31 |

| # | Article | IF | Citations |
|---|---|---|---|
| 653 | Generalized spin-ratio scaled MP2 method for accurate prediction of intermolecular interactions for neutral and ionic species. Journal of Chemical Physics, 2017, 146, 064108. | 1.2 | 34 |
| 654 | Modeling of Sâ€Nitrosothiolâ€“Thiol Reactions of Biological Significance: HNO Production by Sâ€Thiolation Requires a Proton Shuttle and Stabilization of Polar Intermediates. ChemBioChem, 2017, 18, 726-738. | 1.3 | 19 |
| 655 | When does a functional correctly describe both the structure and the energy of the transition state?. Journal of Molecular Modeling, 2017, 23, 65. | 0.8 | 5 |
| 656 | Benzene and Pyridine on Silicon (001): A Trial Ground for Long-Range Corrections in Density Functional Theory. Journal of Physical Chemistry C, 2017, 121, 10484-10500. | 1.5 | 2 |
| 657 | A combined theoretical and experimental study of phenol-(acetylene)n (n â‰¤ 7) clusters. Journal of Chemical Physics, 2017, 146, 154303. | 1.2 | 6 |
| 658 | DFT study of host-dopant systems of DPVBi with organophosphorus Ï€-conjugated materials. Computational and Theoretical Chemistry, 2017, 1113, 61-71. | 1.1 | 3 |
| 659 | Efficient Computation of Exchange Energy Density with Gaussian Basis Functions. Journal of Chemical Theory and Computation, 2017, 13, 2571-2580. | 2.3 | 21 |
| 660 | Adsorption and diffusion of lithium in a graphene/blue-phosphorus heterostructure and the effect of an external electric field. Physical Chemistry Chemical Physics, 2017, 19, 267-275. | 1.3 | 29 |
| 661 | Pyrazole amino acids: hydrogen bonding directed conformations of 3-amino-1H-pyrazole-5-carboxylic acid residue. Journal of Peptide Science, 2017, 23, 716-726. | 0.8 | 2 |
| 662 | Energetics and reactivity of small beryllium deuterides. Journal of Molecular Modeling, 2017, 23, 203. | 0.8 | 6 |
| 663 | Tuning the structural, electronic and electrochemical properties of the 4-methyl-1-phenyl triazolium based [PhMeTAZ][Y 1â€“8 ] ionic liquids through changing anions: A quantum chemical study. Journal of Molecular Liquids, 2017, 240, 138-151. | 2.3 | 13 |
| 664 | Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals. Molecular Physics, 2017, 115, 2315-2372. | 0.8 | 1,401 |
| 665 | Conventional and Explicitly Correlated ab Initio Benchmark Study on Water Clusters: Revision of the BEGDB and WATER27 Data Sets. Journal of Chemical Theory and Computation, 2017, 13, 3136-3152. | 2.3 | 81 |
| 666 | Investigation of polymorphic transitions of piracetam induced during wet granulation. European Journal of Pharmaceutics and Biopharmaceutics, 2017, 119, 36-46. | 2.0 | 10 |
| 667 | DSD-PBEP86-NL and DOD-PBEP86-NL functionals for noncovalent interactions: Basis set effects and tentative applications to large noncovalent systems. International Journal of Quantum Chemistry, 2017, 117, e25417. | 1.0 | 6 |
| 668 | Electrodeposition of Al from chloroaluminate ionic liquids with different cations. Ionics, 2017, 23, 2449-2455. | 1.2 | 19 |
| 669 | Effect of surface roughness on van der Waals and Casimir-Polder/Casimir attraction energies. Surface Science, 2017, 663, 88-99. | 0.8 | 2 |
| 670 | Confinement of hydrogen and hydroxyl radicals in water cages: a density functional theory study. RSC Advances, 2017, 7, 14537-14543. | 1.7 | 5 |

| # | Article | IF | Citations |
|---|---|---|---|
| 671 | Efficient Implementation of Energy Decomposition Analysis for Second-Order MÃ¸llerâ€“Plesset Perturbation Theory and Application to Anionâ^Ï€ Interactions. Journal of Physical Chemistry A, 2017, 121, 717-728. | 1.1 | 30 |
| 672 | Equilibria and Speciation of Chloramines, Bromamines, and Bromochloramines in Water. Environmental Science & Technology, 2017, 51, 128-140. | 4.6 | 26 |
| 673 | Density functional theory for modelling large molecular adsorbateâ€“surface interactions: a mini-review and worked example. Molecular Simulation, 2017, 43, 327-345. | 0.9 | 39 |
| 674 | 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 |
| 675 | Development of a Flexibleâ€Monomer Twoâ€Body Carbon Dioxide Potential and Its Application to Clusters up to (CO<sub>2</sub>)<sub>13</sub>. Journal of Computational Chemistry, 2017, 38, 2763-2774. | 1.5 | 13 |
| 676 | Computational investigations of S 3 structures related to a recent X-ray free electron laser study. Chemical Physics Letters, 2017, 690, 172-176. | 1.2 | 20 |
| 677 | Improving the Efficiency of Beyond-RPA Methods within the Dielectric Matrix Formulation: Algorithms and Applications to the A24 and S22 Test Sets. Journal of Chemical Theory and Computation, 2017, 13, 5432-5442. | 2.3 | 16 |
| 678 | 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 |
| 679 | Exploring the pnicogen bond non-covalent interactions in 4-XPhNH2:PFnH3-n complexes (n = 1â€“3, X = H,) Tj ETQq0 0 0 rgBT /Overloch | 0.9 | 3 |
| 680 | Benchmark Databases of Intermolecular Interaction Energies: Design, Construction, and Significance. Annual Reports in Computational Chemistry, 2017, 13, 3-91. | 0.9 | 8 |
| 681 | Generalized Optimized Effective Potential for Orbital Functionals and Self-Consistent Calculation of Random Phase Approximations. Journal of Physical Chemistry Letters, 2017, 8, 4746-4751. | 2.1 | 18 |
| 683 | General optimization procedure towards the design of a new family of minimal parameter spin-component-scaled double-hybrid density functional theory. Physical Chemistry Chemical Physics, 2017, 19, 26191-26200. | 1.3 | 20 |
| 684 | Aluminum(<scp>i</scp>) Î²-diketiminato complexes activate C(sp<sup>2</sup>)â€“F and C(sp<sup>3</sup>)â€“F bonds by different oxidative addition mechanisms: a DFT study. Chemical Communications, 2017, 53, 8196-8198. | 2.2 | 15 |
| 685 | Assessment of Density Functionals for Computing Thermodynamic Properties of Lanthanide Complexes. ChemPhysChem, 2017, 18, 2688-2696. | 1.0 | 25 |
| 686 | Insight into the Role of Additives in Controlling Polymorphic Outcome: A CO<sub>2</sub>-Antisolvent Crystallization Process of Carbamazepine. Crystal Growth and Design, 2017, 17, 4544-4553. | 1.4 | 49 |
| 687 | Assessment of two hybrid van der Waals density functionals for covalent and non-covalent binding of molecules. Journal of Chemical Physics, 2017, 146, 234106. | 1.2 | 33 |
| 688 | Cluster size convergence for the energetics of the oxygen evolving complex in PSII. Journal of Computational Chemistry, 2017, 38, 2157-2160. | 1.5 | 6 |
| 689 | Validation of density functionals for pancake-bonded Ï€-dimers; dispersion is not enough. Physical Chemistry Chemical Physics, 2017, 19, 24761-24768. | 1.3 | 32 |

| # | Article | IF | Citations |
|---|---|---|---|
| 690 | Assessing accuracy of exchange-correlation functionals for electron affinities. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750052. | 1.8 | 1 |
| 691 | Atmospheric chemistry of CH<sub>3</sub>O: its unimolecular reaction and reactions with H<sub>2</sub>O, NH<sub>3</sub>, and HF. RSC Advances, 2017, 7, 56211-56219. | 1.7 | 11 |
| 692 | Au(I)-Catalyzed Dimerization of Two Alkyne Unitsâ€"Interplay between Butadienyl and Cyclopropenylmethyl Cation: Model Studies and Trapping Experiments. Journal of Organic Chemistry, 2017, 82, 13572-13582. | 1.7 | 12 |
| 693 | Assessment of CCSD(T), MP2, and DFT methods for the calculations of structures and interaction energies of the peptide backbone with water molecules. Chemical Physics Letters, 2017, 687, 23-30. | 1.2 | 11 |
| 694 | Synthesis meets theory: Past, present and future of rational chemistry. Physical Sciences Reviews, 2017, 2, . | 0.8 | 3 |
| 695 | Toward reliable modeling of S-nitrosothiol chemistry: Structure and properties of methyl thionitrite (CH3SNO), an S-nitrosocysteine model. Journal of Chemical Physics, 2017, 147, 044305. | 1.2 | 11 |
| 696 | Stereoelectronic Interactions as a Probe for the Existence of the Intramolecular Î±-Effect. Journal of the American Chemical Society, 2017, 139, 10799-10813. | 6.6 | 66 |
| 697 | Identification and characterization of intramolecular Î³-halo interaction in d0 complexes: a theoretical approach. Journal of Molecular Modeling, 2017, 23, 213. | 0.8 | 1 |
| 698 | Mechanism of the Copper/TEMPOâ€Catalyzed Aerobic Oxidation of Alcohols. Chemistry - A European Journal, 2017, 23, 1368-1378. | 1.7 | 45 |
| 699 | A Comprehensive Overview of the DFT-D3 London-Dispersion Correction. , 2017, , 195-219. | | 57 |
| 700 | Intermolecular Interaction Energies from Kohnâ€"Sham Random Phase Approximation Correlation Methods. , 2017, , 65-136. | | 6 |
| 701 | Cyclic Compounds Incorporating Two or Four Alkyne Units in Close Proximity â€" Theory and Experiments. European Journal of Organic Chemistry, 2018, 2018, 2406-2416. | 1.2 | 3 |
| 702 | Intermolecular dispersion energies from coupled exact-exchange Kohn-Sham excitation energies and vectors. Computational and Theoretical Chemistry, 2018, 1129, 57-69. | 1.1 | 4 |
| 703 | Thiophene Separation with Silver-Doped Cu-BTC Metalâ€"Organic Framework for Deep Desulfurization. Industrial & Engineering Chemistry Research, 2018, 57, 2956-2966. | 1.8 | 25 |
| 704 | Origin of Stereocontrol in Photoredox Organocatalysis of Asymmetric Î±-Functionalizations of Aldehydes. Journal of Organic Chemistry, 2018, 83, 3333-3338. | 1.7 | 11 |
| 705 | Insight into catalytic reduction of CO<sub>2</sub>to methane with silanes using Brookhart's cationic Ir(<scp>iii</scp>) pincer complex. RSC Advances, 2018, 8, 9232-9242. | 1.7 | 11 |
| 706 | Tautomeric preferences of the cis and trans isomers of axitinib. Chemical Physics, 2018, 507, 10-18. | 0.9 | 4 |
| 707 | Crystal Nucleation of Tolbutamide in Solution: Relationship to Solvent, Solute Conformation, and Solution Structure. Chemistry - A European Journal, 2018, 24, 4916-4926. | 1.7 | 49 |

| # | Article | IF | Citations |
|---|---|---|---|
| 708 | Impact of long-range electrostatic and dispersive interactions on theoretical predictions of adsorption and catalysis in zeolites. Catalysis Today, 2018, 312, 51-65. | 2.2 | 35 |
| 709 | Ultrafast stimulated emission of nitrophenolates in organic and aqueous solutions. Physical Chemistry Chemical Physics, 2018, 20, 10713-10720. | 1.3 | 5 |
| 710 | From Noncovalent Chalcogenâ€“Chalcogen Interactions to Supramolecular Aggregates: Experiments and Calculations. Chemical Reviews, 2018, 118, 2010-2041. | 23.0 | 244 |
| 711 | Is there computational support for an unprotonated carbon in the E<sub>4</sub> state of nitrogenase?. Journal of Computational Chemistry, 2018, 39, 743-747. | 1.5 | 28 |
| 712 | Chemistry of oxidomolybdenum(IV) and -(VI) complexes with ONS donor ligands: Synthesis, computational evaluation and oxo-transfer reactions. Polyhedron, 2018, 141, 322-336. | 1.0 | 7 |
| 713 | What Happens Without Nickel? Cyclization Reactions of Ethylene with Ethanedithial and Related Molecules. Journal of Computational Chemistry, 2018, 39, 1158-1167. | 1.5 | 0 |
| 714 | Nitrido complex of high-valent Ru(VI) -catalyzed reduction of imines and alkynes with hydrosilanes: A theoretical study of the reaction mechanism. Journal of Organometallic Chemistry, 2018, 864, 2-11. | 0.8 | 6 |
| 715 | Structural and energetic quantum chemical investigations into how the bioactive thiazolidinedione and rhodanine scaffolds interact with cytosine to form part of DNA. Computational and Theoretical Chemistry, 2018, 1125, 1-14. | 1.1 | 0 |
| 716 | Hirshfeld-based atomic population analysis of the B, N doping effect in zigzag graphene nanoribbons: $$pi$$Ï€ electron density as requirement to follow the B, N doping guidelines. Theoretical Chemistry Accounts, 2018, 137, 1. | 0.5 | 4 |
| 717 | How to tame a palladium terminal imido. Journal of Organometallic Chemistry, 2018, 864, 26-36. | 0.8 | 14 |
| 718 | A Major Structural Change of the Homocitrate Ligand of Probable Importance for the Nitrogenase Mechanism. Inorganic Chemistry, 2018, 57, 1090-1095. | 1.9 | 28 |
| 719 | A general range-separated double-hybrid density-functional theory. Journal of Chemical Physics, 2018, 148, 164105. | 1.2 | 33 |
| 720 | Ozone-Free Synthesis of Ozonides: Assembling Bicyclic Structures from 1,5-Diketones and Hydrogen Peroxide. Journal of Organic Chemistry, 2018, 83, 4402-4426. | 1.7 | 44 |
| 721 | Molecular engineering of the electronic, structural, and electrochemical properties of nanostructured 1-methyl-4-phenyl 1,2,4 triazolium-based [PhMTZ][X1â€“10] ionic liquids through anionic changing. Ionics, 2018, 24, 483-504. | 1.2 | 6 |
| 722 | Adsorption of TNT, DNAN, NTO, FOX7, and NQ onto cellulose, chitin, and cellulose triacetate. Insights from Density Functional Theory calculations. Surface Science, 2018, 668, 54-60. | 0.8 | 14 |
| 723 | A comparative study of the structures and electronic properties of graphene fragments: A DFT and MP2 survey. Chemical Physics Letters, 2018, 691, 291-297. | 1.2 | 5 |
| 724 | Mechanistic insights into the catalytic carbonyl hydrosilylation by cationic [CpM(CO)<sub>2</sub>(IMes)]<sup>+</sup> (M = Mo, W) complexes: the intermediacy of Î·<sup>1</sup>-H(Si) metal complexes. New Journal of Chemistry, 2018, 42, 4923-4932. | 1.4 | 5 |
| 725 | The truth is out there: the metal-Ï€ interactions in crystal of Cr(CO)<sub>3</sub>(pcp) as revealed by the study of vibrational smearing of electron density. Zeitschrift Fur Kristallographie - Crystalline Materials, 2018, 233, 317-336. | 0.4 | 7 |

| # | Article | IF | Citations |
|---|---|---|---|
| 726 | A quantum chemical study of the interactions of uracil as a constituent of ribonucleic acid (RNA) with thiazolidinedione and rhodanine bioactive molecules: an insight into energetic and structural features. Structural Chemistry, 2018, 29, 681-702. | 1.0 | 4 |
| 727 | Substituent effects on gas-phase homolytic Fe–N bond energies of mâ€Câ€<sub>6</sub>H<sub>4</sub>NHFe(CO)<sub>2</sub>(Î·<sup>5</sup>â€<sub>5</sub>H<sub>5</sub>) and mâ€Câ€<sub>6</sub>H<sub>4</sub>N(COMe)Fe(CO)<sub>2</sub>(Î·<sup>5</sup>â€<sub>5</sub>H<sub>5</sub>) studied using density functional theory methods. Journal of Physical Organic Chemistry, 2018, 31, e3782. | 0.9 | 1 |
| 728 | A Systematic DFT Approach for Studying Mechanisms of Redox Active Enzymes. Frontiers in Chemistry, 2018, 6, 644. | 1.8 | 44 |
| 729 | â€˜Diet GMTKN55â€™ offers accelerated benchmarking through a representative subset approach. Physical Chemistry Chemical Physics, 2018, 20, 27735-27739. | 1.3 | 26 |
| 730 | A New 1:1 Drug-Drug Cocrystal of Theophylline and Aspirin: Discovery, Characterization, and Construction of Ternary Phase Diagrams. Crystal Growth and Design, 2018, 18, 7526-7532. | 1.4 | 61 |
| 731 | Roaming-like Mechanism for Dehydration of Diol Radicals. Journal of Physical Chemistry A, 2018, 122, 9738-9754. | 1.1 | 7 |
| 732 | DFT Protocol for EPR Prediction of Paramagnetic Cu(II) Complexes and Application to Protein Binding Sites. Magnetochemistry, 2018, 4, 55. | 1.0 | 30 |
| 733 | The Nonlocal Kernel in van der Waals Density Functionals as an Additive Correction: An Extensive Analysis with Special Emphasis on the B97M-V and ï‰B97M-V Approaches. Journal of Chemical Theory and Computation, 2018, 14, 5725-5738. | 2.3 | 170 |
| 734 | Assessment of a range-separated orbital-optimised random-phase approximation electron correlation method. Theoretical Chemistry Accounts, 2018, 137, 1. | 0.5 | 6 |
| 735 | Organic phototransistors based on perylene diimide nanocrystals lacking Ï€â€“Ï€ interactions. Journal of Materials Chemistry C, 2018, 6, 10597-10602. | 2.7 | 12 |
| 736 | Understanding the role of ethylene glycol in a remarkable catalyst-free Strecker reaction of a-CF3 ketoimine: A theoretical study. Computational and Theoretical Chemistry, 2018, 1142, 57-65. | 1.1 | 0 |
| 737 | Thermodynamic Properties of the Methylmethoxy Radical with Intricate Treatment of Two-Dimensional Hindered Internal Rotations. Journal of Chemical & Engineering Data, 2018, 63, 3640-3649. | 1.0 | 3 |
| 738 | Dimerization of Substituted Arylacetylenesâ€”Quantum Chemical Calculations and Kinetic Studies. Journal of Organic Chemistry, 2018, 83, 7878-7885. | 1.7 | 14 |
| 739 | Exploring conformational preferences of alanine tetrapeptide by CCSD(T), MP2, and dispersion-corrected DFT methods. Chemical Physics Letters, 2018, 702, 69-75. | 1.2 | 12 |
| 740 | Puckering transitions in cyclohexane: Revisited. Chemical Physics Letters, 2018, 702, 82-89. | 1.2 | 9 |
| 741 | Accurate prediction of vertical electronic transitions of Ni(II) coordination compounds via time dependent density functional theory. International Journal of Quantum Chemistry, 2018, 118, e25655. | 1.0 | 16 |
| 742 | A Comprehensive Assessment of the Effectiveness of Orbital Optimization in Double-Hybrid Density Functionals in the Treatment of Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Physical Chemistry A, 2018, 122, 5610-5624. | 1.1 | 19 |
| 743 | Influence of Structurally Related Impurities on the Crystal Nucleation of Curcumin. Crystal Growth and Design, 2018, 18, 4715-4723. | 1.4 | 33 |

| # | Article | IF | Citations |
|---|---|---|---|
| 744 | Semi-empirical or non-empirical double-hybrid density functionals: which are more robust?. Physical Chemistry Chemical Physics, 2018, 20, 23175-23194. | 1.3 | 102 |
| 745 | Shannon Entropy in Atoms: A Test for the Assessment of Density Functionals in Kohn-Sham Theory. Computation, 2018, 6, 36. | 1.0 | 4 |
| 746 | Theoretical Prediction of Blue Phosphorene/Borophene Heterostructure as a Promising Anode Material for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2018, 122, 18294-18303. | 1.5 | 59 |
| 747 | The S<sub>2</sub> to S<sub>3</sub> transition for water oxidation in PSII (photosystem II), revisited. Physical Chemistry Chemical Physics, 2018, 20, 22926-22931. | 1.3 | 61 |
| 748 | Linear tricationic ionic liquids: Insights into the structural features using DFT and molecular dynamics simulation. Journal of Molecular Liquids, 2018, 271, 96-104. | 2.3 | 17 |
| 749 | Evaluation of Common Theoretical Methods for Predicting Infrared Multiphotonic Dissociation Vibrational Spectra of Intramolecular Hydrogen-Bonded Ions. ACS Omega, 2018, 3, 9075-9085. | 1.6 | 38 |
| 750 | Pâ€Stereogenic PN(H)P Iron(II) Catalysts for the Asymmetric Hydrogenation of Ketones: The Importance of Nonâ€Covalent Interactions in Rational Ligand Design by Computation. Advanced Synthesis and Catalysis, 2018, 360, 2900-2913. | 2.1 | 33 |
| 751 | Theoretical studies of atmospheric molecular complexes interacting with NIR to UV light. Faraday Discussions, 2018, 212, 421-441. | 1.6 | 7 |
| 752 | Survival of the most transferable at the top of Jacobâ€™s ladder: Defining and testing the Ï‰B97M(2) double hybrid density functional. Journal of Chemical Physics, 2018, 148, 241736. | 1.2 | 136 |
| 753 | On the formation of propylene oxide from propylene in space: gas-phase reactions. Theoretical Chemistry Accounts, 2019, 138, 1. | 0.5 | 3 |
| 754 | Cost-effective density functional theory (DFT) calculations of equilibrium isotopic fractionation in large organic molecules. Physical Chemistry Chemical Physics, 2019, 21, 17555-17570. | 1.3 | 11 |
| 755 | Calculations of the relative populations of Lu@C<sub>82</sub> isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2019, 27, 710-714. | 1.0 | 10 |
| 756 | Exploration of the basic reactant in CO2 photoreduction: New insights from photophysics and photochemistry. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 382, 111959. | 2.0 | 2 |
| 757 | Annular Tautomerism of 3(5)-Disubstituted-1H-pyrazoles with Ester and Amide Groups. Molecules, 2019, 24, 2632. | 1.7 | 12 |
| 758 | Quantum-mechanical study of energies, structures and vibrational spectra of the HF complexed with dimethyl ether. Chemical Physics Letters, 2019, 731, 136590. | 1.2 | 2 |
| 759 | Structural and photophysical studies of triphenylamine-based nonlinear optical dyes: effects of Ï€-linker moieties on the D-Ï€-A structure. Comptes Rendus Chimie, 2019, 22, 373-385. | 0.2 | 10 |
| 760 | Chalcogenide glasses as a playground for the application of first-principles molecular dynamics to disordered materials. Solid State Sciences, 2019, 95, 105925. | 1.5 | 4 |
| 761 | Locality and strength of intermolecular interactions in organic crystals: using conceptual density functional theory (CDFT) to characterize a highly polymorphic system. Theoretical Chemistry Accounts, 2019, 138, 1. | 0.5 | 3 |

| # | Article | IF | Citations |
|---|---|---|---|
| 762 | Computational investigation on the reaction of dimethyl ether with nitric dioxide. I. Underlying mechanism and accurate energetics. Theoretical Chemistry Accounts, 2019, 138, 1. | 0.5 | 4 |
| 763 | Investigation on the Thermal Dissociation of Vinyl Nitrite with a Saddle Point Involved. ACS Omega, 2019, 4, 16052-16061. | 1.6 | 2 |
| 764 | Revisiting the Potential Energy Surface of the Stacked Cytosine Dimer: FNO-CCSD(T) Interaction Energies, SAPT Decompositions, and Benchmarking. Journal of Physical Chemistry A, 2019, 123, 9209-9222. | 1.1 | 9 |
| 765 | Racemization of oxazepam and chiral 1,4-benzodiazepines. DFT study of the reaction mechanism in aqueous solution. Organic and Biomolecular Chemistry, 2019, 17, 1471-1479. | 1.5 | 11 |
| 766 | Implementation of the Many-Pair Expansion for Systematically Improving Density Functional Calculations of Molecules. Journal of Chemical Theory and Computation, 2019, 15, 1089-1101. | 2.3 | 5 |
| 767 | Iodine-Catalyzed Nazarov Cyclizations. Journal of Organic Chemistry, 2019, 84, 7587-7605. | 1.7 | 32 |
| 768 | Does (H5O2)+â^' X (Xâ€¯=â€¯Ar, Ne, He) complex with C2 symmetry really exist?. Journal of Molecular Liquids, 2019, 288, 111075. | 2.3 | 1 |
| 769 | Thermal degradation of formamidinium based lead halide perovskites into sym-triazine and hydrogen cyanide observed by coupled thermogravimetry-mass spectrometry analysis. Journal of Materials Chemistry A, 2019, 7, 16912-16919. | 5.2 | 163 |
| 770 | Calculated relative populations for the Eu@C82 isomers. Chemical Physics Letters, 2019, 726, 29-33. | 1.2 | 13 |
| 771 | Infrared Spectroscopy and Mass Spectrometry of CO<sub>2</sub> Clusters during Nucleation and Growth. Journal of Physical Chemistry A, 2019, 123, 2426-2437. | 1.1 | 14 |
| 772 | DFT Computed Dielectric Response and THz Spectra of Organic Co-Crystals and Their Constituent Components. Molecules, 2019, 24, 959. | 1.7 | 2 |
| 773 | Electronic Relaxation Dynamics of UV-Photoexcited 2-Aminopurineâ€“Thymine Base Pairs in Watsonâ€“Crick and Hoogsteen Conformations. Journal of Physical Chemistry B, 2019, 123, 2904-2914. | 1.2 | 7 |
| 774 | DFT study on selective autocatalyzed <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mi>Î±</mml:mi></mml:mrow></mml:math>-alkylation of ketones with alcohols. Journal of Catalysis, 2019, 373, 126-138. | 3.1 | 6 |
| 775 | Evaluating Transition Metal Barrier Heights with the Latest Density Functional Theory Exchangeâ€“Correlation Functionals: The MOBH35 Benchmark Database. Journal of Physical Chemistry A, 2019, 123, 3761-3781. | 1.1 | 104 |
| 776 | Semiempirical Quantum-Chemical Methods with Orthogonalization and Dispersion Corrections. Journal of Chemical Theory and Computation, 2019, 15, 1743-1760. | 2.3 | 45 |
| 777 | Dimerization of substituted 4-aryl-1,3-diacetylenes â€“ quantum chemical calculations and kinetic studies. Organic Chemistry Frontiers, 2019, 6, 1010-1021. | 2.3 | 9 |
| 778 | Effect of the exchangeâ€“correlation functional on the synchronicity/nonsynchronicity in bond formation in Dielsâ€“Alder reactions: a reaction force constant analysis. Physical Chemistry Chemical Physics, 2019, 21, 7412-7428. | 1.3 | 31 |
| 779 | Capturing a Square Planar Gold(III) Complex Inside a Platinum Nanocage: A Combined Experimental and Theoretical Study. Inorganic Chemistry, 2019, 58, 3189-3195. | 1.9 | 19 |

| # | Article | IF | Citations |
|---|---|---|---|
| 780 | Computational Modeling of the Ce@C<sub>82</sub> Metallofullerene Isomeric Composition. ECS Journal of Solid State Science and Technology, 2019, 8, M118-M121. | 0.9 | 9 |
| 781 | ACCDB: A collection of chemistry databases for broad computational purposes. Journal of Computational Chemistry, 2019, 40, 839-848. | 1.5 | 42 |
| 782 | Direct measurements of C<sub>3</sub>F<sub>7</sub>I dissociation rate constants using a shock tube ARAS technique. International Journal of Chemical Kinetics, 2019, 51, 206-214. | 1.0 | 4 |
| 783 | Evaluating Density Functionals by Examining Molecular Structures, Chemical Bonding, and Relative Energies of Mononuclear Ruâ€“Clâ€“Hâ€“PR3 Isomers. Journal of Physical Chemistry A, 2019, 123, 343-358. | 1.1 | 1 |
| 784 | Unraveling the Link between Solvent-Mediated Proton Transfer and the Salt Formation of Saccharin and Sulfamethazine. Crystal Growth and Design, 2019, 19, 613-619. | 1.4 | 7 |
| 785 | Theoretical study of the mechanism of the manganese catalase KatB. Journal of Biological Inorganic Chemistry, 2019, 24, 103-115. | 1.1 | 4 |
| 786 | Anharmonicity of the bonded O H group vibrations in water dimer. DFT study including dispersion interaction. Journal of Molecular Liquids, 2019, 277, 269-279. | 2.3 | 5 |
| 787 | Generalized Kohnâ€Sham energy decomposition analysis and its applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1460. | 6.2 | 55 |
| 788 | Hindered rotational barriers in conjugated donorâ€“acceptor substituted systems: calculations vs. experiments. Physical Chemistry Chemical Physics, 2020, 22, 1214-1221. | 1.3 | 4 |
| 789 | Substituent effects on the halogen and pnictogen bonds characteristics in ternary complexes 4-YPhNH2Â·Â·Â·PH2FÂ·Â·Â·ClX (Yâ€‰=â€‰H, F, CN, CHO, NH2, CH3, NO2 and OCH3, and Xâ€‰=â€‰F, OH, CN, NC, FCC and NO2): theoretical study. Journal of Chemical Sciences, 2020, 132, 1. | 1.1 | 11 |
| 790 | A computational study of the interaction of C2 hydrocarbons with CuBTC. Computational Materials Science, 2020, 173, 109438. | 1.4 | 5 |
| 791 | Study of the mechanisms of dialkyl carbonates directly formed from carbon dioxide and alcohols: New insights from kinetic and thermodynamic processes. Molecular Catalysis, 2020, 482, 110699. | 1.0 | 2 |
| 792 | Quantitative prediction of electronic absorption spectra of copper(II)â€“bioligand systems: Validation and applications. Journal of Inorganic Biochemistry, 2020, 204, 110953. | 1.5 | 27 |
| 793 | Density Functional Theory as a Data Science. Chemical Record, 2020, 20, 618-639. | 2.9 | 9 |
| 794 | Empirical Doubleâ€Hybrid Density Functional Theory: A â€˜Third Wayâ€™ in Between WFT and DFT. Israel Journal of Chemistry, 2020, 60, 787-804. | 1.0 | 129 |
| 795 | Conformational preferences of cationic Î²-peptide in water studied by CCSD(T), MP2, and DFT methods. Heliyon, 2020, 6, e04721. | 1.4 | 4 |
| 796 | Investigation of solute-solvent interactions in binary and quaternary solutions containing lithium perchlorate, propylene carbonate, and the deep eutectic solvent (choline chloride/ethylene glycol) at T=(288.15 to 318.15) K. Journal of Molecular Liquids, 2020, 319, 114090. | 2.3 | 8 |
| 797 | A Local Hybrid Functional with Wide Applicability and Good Balance between (De)Localization and Leftâ€“Right Correlation. Journal of Chemical Theory and Computation, 2020, 16, 5645-5657. | 2.3 | 54 |

| # | Article | IF | Citations |
|---|---|---|---|
| 798 | Ho<sub>2</sub>O@D<sub>3</sub>(85)-C<sub>92</sub>: Highly Stretched Cluster Dictated by a Giant Cage and Unexplored Isomerization. Inorganic Chemistry, 2020, 59, 11020-11027. | 1.9 | 12 |
| 799 | Density Functional Theories and Coordination Chemistry. , 2020, , . | | 2 |
| 800 | Structure functionality relationship of flavonoids (myricetin, morin, taxifolin and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 667 Td (3â€²,4â€ Structure, 2020, 1222, 128923. | 1.8 | 3 |
| 801 | Adsorption of cytarabine and gemcitabine anticancer drugs on the BNNT surface: DFT and GD3-DFT approaches. Adsorption, 2020, 26, 1365-1384. | 1.4 | 5 |
| 802 | Structure, Stability, and Spectroscopic Properties of Small Acetonitrile Cation Clusters. Journal of Physical Chemistry A, 2020, 124, 6845-6855. | 1.1 | 6 |
| 803 | Monomolecular decomposition of C<sub>3</sub>F<sub>7</sub>I and CF<sub>3</sub>I: Theory meets experiment. Journal of Physics: Conference Series, 2020, 1556, 012037. | 0.3 | 1 |
| 804 | Synthesis of Trialkylamines with Extreme Steric Hindrance and Their Decay by a Hofmann-like Elimination Reaction. Journal of Organic Chemistry, 2020, 85, 13630-13643. | 1.7 | 5 |
| 805 | On the Kinetic Mechanism of Ignition of Diborane Mixtures with Air. Combustion, Explosion and Shock Waves, 2020, 56, 249-266. | 0.3 | 5 |
| 806 | Accuracy of intermolecular interaction energies, particularly those of hetero-atom containing molecules obtained by DFT calculations with Grimme's D2, D3 and D3BJ dispersion corrections. Physical Chemistry Chemical Physics, 2020, 22, 22508-22519. | 1.3 | 68 |
| 807 | Efficient yet accurate dispersion-corrected semilocal exchangeâ€“correlation functionals for non-covalent interactions. Journal of Chemical Physics, 2020, 153, 084117. | 1.2 | 10 |
| 808 | Adsorption and dissociation of molecular hydrogen on Na3Al5 and Na5Al5 clusters. Chemical Physics Letters, 2020, 758, 137922. | 1.2 | 3 |
| 809 | Toward accurate prediction of amino acid derivatives structure and energetics from DFT: glycine conformers and their interconversions. Journal of Molecular Modeling, 2020, 26, 129. | 0.8 | 15 |
| 810 | Improving Tabletability of Excipients by Metal-Organic Framework-Based Cocrystallization: a Study of Mannitol and CaCl2. Pharmaceutical Research, 2020, 37, 130. | 1.7 | 12 |
| 811 | Multiâ€coefficients correlation methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1474. | 6.2 | 4 |
| 812 | Global uncertainty analysis for the RRKM/master equation modeling of a typical multi-well and multi-channel reaction system. Combustion and Flame, 2020, 216, 62-71. | 2.8 | 13 |
| 813 | Mechanism of Phosphine-Catalyzed Novel Rearrangement of Vinylcyclopropylketone to Cycloheptenone: A DFT Study. ACS Omega, 2020, 5, 2957-2966. | 1.6 | 6 |
| 814 | Eu@C86 isomers: Calculated relative populations. Fullerenes Nanotubes and Carbon Nanostructures, 2020, 28, 565-570. | 1.0 | 7 |
| 815 | A novel contrast of the reactions of 2,4,6-trinitrotoluene (TNT) in atmospheric-pressure O2 and N2 plasma: Experimental and theoretical study. International Journal of Mass Spectrometry, 2020, 450, 116308. | 0.7 | 5 |

| # | Article | IF | Citations |
|---|---|---|---|
| 816 | Electronic-level insight into the weak interactions of ion pairs in acetate anion-based ionic liquids. Journal of Molecular Liquids, 2020, 303, 112668. | 2.3 | 10 |
| 817 | Dualâ€hybrid direct random phase approximation and secondâ€order screened exchange with nonlocal van der Waals correlations for noncovalent interactions. Journal of Computational Chemistry, 2020, 41, 1018-1025. | 1.5 | 0 |
| 818 | Modelling Enzymatic Mechanisms with QM/MM Approaches: Current Status and Future Challenges. Israel Journal of Chemistry, 2020, 60, 655-666. | 1.0 | 40 |
| 819 | Mechanistic Insights into the Chemoâ€Selective Dehydrogenative Silylation of Alkenes Catalyzed by Bis(imino)pyridine Cobalt Complex from DFT Computations. ChemCatChem, 2020, 12, 3890-3899. | 1.8 | 2 |
| 820 | A new database and benchmark of the bond energies of <scp>nobleâ€gas</scp>â€containing molecules. International Journal of Quantum Chemistry, 2020, 120, e26238. | 1.0 | 6 |
| 821 | Vaporâ€“Liquid Equilibria and Computational Study for Aqueous Solutions of Novel Deep Eutectic Solvents (Amino Acid/Lactic Acid) at 298.15 K. Journal of Chemical & Engineering Data, 2020, 65, 3262-3269. | 1.0 | 10 |
| 822 | Theoretical rationalization for the equilibrium between (Î¼â€“Î·<sup>2</sup>:Î·<sup>2</sup>-peroxido)Cu<sup>II</sup>Cu<sup>II</sup> and bis(Î¼-oxido)Cu<sup>III</sup>Cu<sup>III</sup> complexes: perturbational effects from ligand frameworks. Dalton Transactions, 2020, 49, 6710-6717. | 1.6 | 3 |
| 823 | Double hybrid <scp>DFT</scp> calculations with Slater type orbitals. Journal of Computational Chemistry, 2020, 41, 1660-1684. | 1.5 | 16 |
| 824 | Computation of covalent and noncovalent structural parameters at low computational cost: Efficiency of the <scp>DHâ€SVPD</scp> method. International Journal of Quantum Chemistry, 2020, 120, e26233. | 1.0 | 7 |
| 825 | Theoretical studies on how to tune the Ï€â€hole pnicogen bonds by substitution and cooperative effects. International Journal of Quantum Chemistry, 2021, 121, e26531. | 1.0 | 7 |
| 826 | The interplay between anion-Ï€ and H-bonding interactions in Xâ^'Â·Â·Â·s-TriazineÂ·Â·Â·(HF)n(HCl)3-n (Xâ€‰=â€‰F, Clâ^') | 0.8 | 0 |
| 827 | Thermodynamic and computational study of paracetamol in aqueous solutions of some sustainable amino acid-based ionic liquids. Journal of Chemical Thermodynamics, 2021, 155, 106348. | 1.0 | 9 |
| 828 | Stacking interactions in cavity-containing molecular structures built from acylphloroglucinols: a computational study. Molecular Physics, 2021, 119, e1800852. | 0.8 | 2 |
| 829 | Calculated relative populations for the Eu@C84 isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2021, 29, 144-148. | 1.0 | 5 |
| 830 | Critical benchmarking of popular composite thermochemistry models and density functional approximations on a probabilistically pruned benchmark dataset of formation enthalpies. Journal of Chemical Physics, 2021, 154, 044113. | 1.2 | 10 |
| 831 | Electronic and geometric determinants of adsorption: fundamentals and applications. JPhys Energy, 2021, 3, 022001. | 2.3 | 18 |
| 832 | Assessing the Applicability of the Geometric Counterpoise Correction in B2PLYP/Double-Î¶ Calculations for Thermochemistry, Kinetics, and Noncovalent Interactions*. Australian Journal of Chemistry, 2021, , . | 0.5 | 2 |
| 833 | Pairing double hybrid functionals with a tailored basis set for an accurate thermochemistry of hydrocarbons. RSC Advances, 2021, 11, 26073-26082. | 1.7 | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 834 | Insights into the existing form of glycolaldehyde in methanol solution: an experimental and theoretical investigation. New Journal of Chemistry, 2021, 45, 8149-8154. | 1.4 | 2 |
| 835 | How many shades of grey? On the proximity of density functional approximation to ab initio method via calculations of electric multipole moments. Journal of Physics: Conference Series, 2021, 1730, 012126. | 0.3 | 0 |
| 836 | Computational Coordination Chemistry. , 2021, , 241-255. | | 4 |
| 837 | Replacing hybrid density functional theory: motivation and recent advances. Chemical Society Reviews, 2021, 50, 8470-8495. | 18.7 | 80 |
| 838 | The effect of the reagents nature on nucleophilic addition of acetylenes to the C=N bond of aldimines: a quantum-chemical investigation. Journal of Physics: Conference Series, 2021, 1847, 012059. | 0.3 | 0 |
| 839 | Mechanistic Insights into the Dicopper-Complex-Catalyzed Hydroxylation of Methane and Benzene Using Nitric Oxide: A DFT Study. Inorganic Chemistry, 2021, 60, 4599-4609. | 1.9 | 4 |
| 840 | Accurate Receptor-Ligand Binding Free Energies from Fast QM Conformational Chemical Space Sampling. International Journal of Molecular Sciences, 2021, 22, 3078. | 1.8 | 14 |
| 841 | CHAL336 Benchmark Set: How Well Do Quantum-Chemical Methods Describe Chalcogen-Bonding Interactions?. Journal of Chemical Theory and Computation, 2021, 17, 2783-2806. | 2.3 | 42 |
| 842 | Noncovalent Interactions from Models for the MÃ¸llerâ€“Plesset Adiabatic Connection. Journal of Physical Chemistry Letters, 2021, 12, 4867-4875. | 2.1 | 15 |
| 843 | Aldol Condensation Versus Superbase-Catalyzed Addition of Ketones to Acetylenes: A Quantum-Chemical and Experimental Study. Journal of Organic Chemistry, 2021, 86, 7439-7449. | 1.7 | 6 |
| 844 | Iodineâ€Catalyzed Dielsâ€Alder Reactions. ChemCatChem, 2021, 13, 2922-2930. | 1.8 | 12 |
| 845 | A density functional theory study of the hydride shift in the Eschweilerâ€“Clarke reaction. Journal of Physical Organic Chemistry, 2021, 34, e4253. | 0.9 | 0 |
| 846 | A computational characterization of H<sub>2</sub>O<sub>2</sub>@C<sub>60</sub>. Fullerenes Nanotubes and Carbon Nanostructures, 2022, 30, 258-262. | 1.0 | 2 |
| 847 | Initial Thermal Decomposition Mechanism of (NH<sub>2</sub>)<sub>2</sub>Câ•C(NO<sub>2</sub>)(ONO) Revealed by Double-Hybrid Density Functional Calculations. ACS Omega, 2021, 6, 15292-15299. | 1.6 | 3 |
| 848 | Role of Dispersion Interactions in Endohedral TM@(ZnS)12 Structures. ACS Omega, 2021, 6, 16612-16622. | 1.6 | 0 |
| 849 | Laboratory Detection of Cyanoacetic Acid: A Jet-cooled Rotational Study. Astrophysical Journal, 2021, 915, 76. | 1.6 | 4 |
| 850 | Calculated Relative Thermodynamic Stabilities of the Gd@C<sub>82</sub> Isomers. ECS Journal of Solid State Science and Technology, 2021, 10, 071013. | 0.9 | 8 |
| 851 | Examination of How Well Long-Range-Corrected Density Functionals Satisfy the Ionization Energy Theorem. Journal of Chemical Theory and Computation, 2021, 17, 4823-4830. | 2.3 | 17 |

| # | Article | IF | Citations |
|---|---|---|---|
| 852 | Density Functional Theory for Electrocatalysis. Energy and Environmental Materials, 2022, 5, 157-185. | 7.3 | 95 |
| 853 | Extraterrestrial Organic Molecules from [SiX]+ Ions: A Coupled Cluster Theory Inquest for Plausible Reaction Pathways. ACS Earth and Space Chemistry, 2021, 5, 2086-2093. | 1.2 | 0 |
| 854 | Computational Study of the Effect of Doping with Ti on NaAlH4 Nanocluster Dehydrogenation. Russian Journal of Physical Chemistry A, 2021, 95, 1646-1654. | 0.1 | 0 |
| 855 | Tautomeric equilibrium, proton affinity and mass spectrometry fragmentation of flexible hydrogen-bonded precursors and rigid $$hbox {N}longrightarrow hbox {BF}_2$$ fluorescent dyes. Scientific Reports, 2021, 11, 15995. | 1.6 | 2 |
| 856 | Theoretical and experimental study of IR spectra of large phenol-acetylene clusters, Ph(Ac)n for 8 â‰¤ n â‰¤ 12. Journal of the Indian Chemical Society, 2021, 98, 100100. | 1.3 | 2 |
| 857 | Relative energetics of CH3CH2O, CH3CHOH, and CH2CH2OH radical products from ethanol dehydrogenation. Journal of Chemical Physics, 2021, 155, 114306. | 1.2 | 1 |
| 858 | Some thermodynamic properties and computational study of DESs (choline chloride/ethylene glycol) Tj ETQq0 0 0 rgBT /Overlock 10 Tf<br>Journal of Chemical Thermodynamics, 2022, 165, 106642. | 1.0 | 5 |
| 859 | Density Functional Calculations Based on the Exponential Ansatz. Journal of Physical Chemistry A, 2021, 125, 8751-8763. | 1.1 | 2 |
| 860 | Effect of choline chloride based deep eutectic solvents on lithium perchlorateÂ+Âpropylene carbonate solutions: Thermodynamic, transport, electrochemical and computational study. Journal of the Taiwan Institute of Chemical Engineers, 2021, 128, 20-29. | 2.7 | 2 |
| 861 | Quantification and understanding of non-covalent interactions in molecular and ionic systems: Dispersion interactions and hydrogen bonding analysed by thermodynamic methods. Journal of Molecular Liquids, 2021, 343, 117547. | 2.3 | 13 |
| 862 | A comprehensive theoretical analysis of Curtius rearrangement of syn-syn and syn-anti conformers of oxalyl diazide. Journal of Molecular Graphics and Modelling, 2021, 109, 108012. | 1.3 | 1 |
| 863 | Sterics, the core of intermolecular interactions. , 2021, , 1-38. | | 0 |
| 864 | Cycloaddition mechanisms of CO<sub>2</sub> and epoxide catalyzed by salophen â€“ an organocatalyst free from metals and halides. Catalysis Science and Technology, 2021, 11, 2529-2539. | 2.1 | 8 |
| 865 | Realization of the Zn<sup>3+</sup> oxidation state. Nanoscale, 2021, 13, 14041-14048. | 2.8 | 13 |
| 867 | Unraveling the Mechanisms of Ribozyme Catalysis with Multiscale Simulations. Challenges and Advances in Computational Chemistry and Physics, 2009, , 377-408. | 0.6 | 1 |
| 868 | Density Functional Calculations. , 2016, , 483-563. | | 1 |
| 869 | A New Generation of Doubly Hybrid Density Functionals (DHDFs). Springer Briefs in Molecular Science, 2014, , 25-45. | 0.1 | 2 |
| 870 | Coupled Cluster Calculations: Ovos as an Alternative Avenue Towards Treating Still Larger Molecules. Challenges and Advances in Computational Chemistry and Physics, 2010, , 429-454. | 0.6 | 3 |

| # | Article | IF | Citations |
|---|---|---|---|
| 871 | Low-Scaling Tensor Hypercontraction in the Cholesky Molecular Orbital Basis Applied to Second-Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2021, 17, 211-221. | 2.3 | 11 |
| 872 | Chapter 11. Water Oxidation by PSII: A Quantum Chemical Approach. Chemical Biology, 0, , 273-295. | 0.1 | 1 |
| 873 | Formation of interstellar cyanoacetamide: a rotational and computational study. Astronomy and Astrophysics, 2020, 644, A3. | 2.1 | 4 |
| 874 | Theoretical Background of the Fragment Molecular Orbital (FMO) Method and Its Implementation in GAMESS. , 2009, , 5-36. | | 18 |
| 875 | Assessment of the Performance of B2PLYP-D for Describing Intramolecular Ï€-Ï€ and Ïƒ-Ï€ Interactions. Bulletin of the Korean Chemical Society, 2011, 32, 4195-4198. | 1.0 | 5 |
| 876 | 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 |
| 877 | Structural and Vibrational Properties of Amino Acids from Composite Schemes and Double-Hybrid DFT: Hydrogen Bonding in Serine as a Test Case. Journal of Physical Chemistry A, 2021, 125, 9099-9114. | 1.1 | 9 |
| 878 | Structure and IR Spectroscopic Properties of HNCO Complexes with SO2 Isolated in Solid Argon. Molecules, 2021, 26, 6441. | 1.7 | 2 |
| 879 | Combined QM/MM methods for the simulation of condensed phase processes using an approximate DFT approach. Challenges and Advances in Computational Chemistry and Physics, 2008, , 381-405. | 0.6 | 0 |
| 880 | Electron correlation methods based on the random phase approximation. , 2012, , 103-120. | | 0 |
| 881 | Formation of Van Der Waals Complexes in Concerted Unimolecular Elimination Processes. , 2012, 2012, 1-7. | | 1 |
| 882 | Ï€-Stacking on Density Functional Theory: A Review. , 2014, , 245-270. | | 1 |
| 883 | Benchmarking the Performance of DHDFs for the Main Group Chemistry. Springer Briefs in Molecular Science, 2014, , 47-77. | 0.1 | 0 |
| 884 | Corrections for Functionals. , 2014, , 125-160. | | 0 |
| 886 | Highly conductive MWNT/silicone composite with low density MWNT bundles. International Symposium on Microelectronics, 2015, 2015, 000638-000643. | 0.3 | 0 |
| 888 | Rotameric Isomers of La<sub>2</sub>@C<sub>80</sub> & Dodecafluoro-Subphthalocyanine Conjugate: Computational Characterization. ECS Journal of Solid State Science and Technology, 2020, 9, 061014. | 0.9 | 6 |
| 890 | Structural and Energetic Properties of Amino Acids and Peptides Benchmarked by Accurate Theoretical and Experimental Data. Journal of Physical Chemistry A, 2021, 125, 9826-9837. | 1.1 | 6 |
| 891 | Correlation Effects in Trimeric Acylphloroglucinols. Computation, 2021, 9, 121. | 1.0 | 5 |

| # | Article | IF | Citations |
|---|---|---|---|
| 892 | Estimation of electron absorption spectra and lifetime of the two lowest singlet excited states of pyrimidine nucleobases and their derivatives. Journal of Molecular Structure, 2021, 1250, 131863. | 1.8 | 4 |
| 893 | The ground and ionized states of azulene: A combined study of the vibrational energy levels by photoionization, configuration interaction, and density functional calculations. Journal of Chemical Physics, 2022, 156, 064305. | 1.2 | 2 |
| 894 | Dispersion size-consistency. Electronic Structure, 2022, 4, 014003. | 1.0 | 3 |
| 895 | Matrix Isolation FTIR and Theoretical Study of Weakly Bound Complexes of Isocyanic Acid with Nitrogen. Molecules, 2022, 27, 495. | 1.7 | 5 |
| 896 | A general justification for hybrid functionals in DFT by means of linear response theory*. Journal of Physics Condensed Matter, 2022, 34, 194004. | 0.7 | 0 |
| 897 | Density Functional Theory for Transition Metal Catalysis. , 2024, , 562-585. | | 0 |
| 898 | Mechanistic study on reduction of nitric oxide to nitrous oxide using a dicopper complex. Dalton Transactions, 2022, 51, 5399-5403. | 1.6 | 1 |
| 899 | Strain and external electric field modulation of the electronic and optical properties of GaN/WSe2 vdWHs. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 142, 115258. | 1.3 | 16 |
| 900 | Incorporation of Different Metal Ion for Tuning Color and Enhancing Antioxidant Activity of Curcumin/Palygorskite Hybrid Materials. Frontiers in Chemistry, 2021, 9, 760941. | 1.8 | 6 |
| 901 | Generation of Phenol and Molecular Hydrogen through Catalyst-Free Câ€“H Activation of Benzene by Water Radical Cations. Journal of the American Society for Mass Spectrometry, 2022, 33, 68-73. | 1.2 | 7 |
| 902 | Small-Basis Set Density-Functional Theory Methods Corrected with Atom-Centered Potentials. Journal of Chemical Theory and Computation, 2022, 18, 2913-2930. | 2.3 | 4 |
| 903 | Superhalogen Anions Supported by the Systems Comprising Alternately Aligned Boron and Nitrogen Central Atoms. Frontiers in Chemistry, 2022, 10, 863408. | 1.8 | 3 |
| 904 | Double Hybrids and Noncovalent Interactions: How Far Can We Go?. Journal of Physical Chemistry A, 2022, 126, 2590-2599. | 1.1 | 9 |
| 905 | Effect of new DFT methods on spectroscopy and NLO analysis of 2-Bromo-5-nitrothiozole and nitrosodimethylamine. Journal of Molecular Modeling, 2022, 28, 135. | 0.8 | 0 |
| 906 | Conformational preferences and intramolecular hydrogen bonding patterns of tetraflavaspidic acid BBBB â€“ a tetrameric acylphloroglucinol. ChemistrySelect, 2022, . | 0.7 | 0 |
| 907 | Weakly Bound Complex Formation between HCN and CH<sub>3</sub>Cl: A Matrix-Isolation and Computational Study. Journal of Physical Chemistry A, 2022, 126, 3110-3123. | 1.1 | 4 |
| 908 | Theoretical mechanistic insights into the polar hydrohalogenation of olefins. Organic and Biomolecular Chemistry, 2022, 20, 4976-4985. | 1.5 | 2 |
| 909 | Quantum Chemical Calculation on the Decomposition Mechanism of Na3AlF6. Russian Journal of Physical Chemistry A, 2022, 96, 1035-1043. | 0.1 | 2 |

| # | Article | IF | Citations |
|---|---|---|---|
| 910 | A theoretical analysis on the electron and energy transfer between host and guest materials in phosphorâ€“doped OLED. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 432, 114058. | 2.0 | 2 |
| 911 | Peat-derived nitrogen-doped porous carbons as photothermal-assisted visible-light photocatalysts for water splitting. New Carbon Materials, 2022, 37, 585-594. | 2.9 | 3 |
| 912 | Analytic Gradients for the Long-Range-Corrected XYG3 Type of Doubly Hybrid Density Functionals: Theory, Implementation, and Assessment. Journal of Physical Chemistry A, 2022, 126, 3937-3946. | 1.1 | 1 |
| 913 | Density Functional Theory Study on the Electronic, Optical and Adsorption Properties of Ti-, Fe- and Ni- Doped Graphene. SSRN Electronic Journal, 0, , . | 0.4 | 0 |
| 914 | Experimental studies on thermophysical properties of protic ionic liquids for thermal energy storage systems. Journal of Energy Storage, 2022, 54, 105251. | 3.9 | 15 |
| 915 | Mechanistic Insights into Criegee Intermediateâ€“Hydroperoxyl Radical Chemistry. Journal of the American Chemical Society, 2022, 144, 14740-14747. | 6.6 | 3 |
| 916 | Verification of the Accuracy and Efficiency of Dispersion-Corrected Density Functional Theory Methods to Describe the Lattice Structure and Energy of Energetic Cocrystals. Crystal Growth and Design, 2022, 22, 5307-5321. | 1.4 | 5 |
| 917 | Density functional theory study on the electronic, optical and adsorption properties of Ti-, Fe- and Ni-doped graphene. Diamond and Related Materials, 2022, 128, 109290. | 1.8 | 6 |
| 918 | Antimony(III)-selenium complexes with synergetic effect between Sb Se bond and Sbâ‹¯Ï€ interactions. Polyhedron, 2022, 225, 116069. | 1.0 | 0 |
| 919 | Two-dimensional GaS/MoTe2 van der Waals heterostructures with tunable electronic and optical properties. Materials Science in Semiconductor Processing, 2022, 152, 107103. | 1.9 | 4 |
| 920 | SiC2/BP5: A pentagonal van der Waals heterostructure with tunable optoelectronic and mechanical properties. Applied Surface Science, 2022, 606, 154857. | 3.1 | 2 |
| 921 | Sic2/Bp5: A Pentagonal Van Der Waals Heterostructure with Tunable Optoelectronic and Mechanical Properties. SSRN Electronic Journal, 0, , . | 0.4 | 0 |
| 922 | Theoretical Predictions of Fullerene Stabilities. , 2022, , 111-179. | | 1 |
| 923 | Intramolecular Hydrogen Bonding Patterns and Conformational Preferences of Ouabainâ€”A Molecule with Cardiotonic and Antiviral Activities. Engineering Materials, 2022, , 671-696. | 0.3 | 0 |
| 924 | Semistabilized Diazatrienyl Anions from Pyridine Imines and Acetylenes: An Access to (Z)-Stilbene/Imidazopyridine Ensembles, Benzyl Imidazopyridines, and Beyond. Journal of Organic Chemistry, 2022, 87, 12225-12239. | 1.7 | 8 |
| 925 | Unveiling the Shape of N-Acetylgalactosamine: A Cancer-Associated Sugar Derivative. Journal of Physical Chemistry A, 2022, 126, 7621-7626. | 1.1 | 1 |
| 926 | Explicitly Correlated Double-Hybrid DFT: A Comprehensive Analysis of the Basis Set Convergence on the GMTKN55 Database. Journal of Chemical Theory and Computation, 2022, 18, 5978-5991. | 2.3 | 15 |
| 927 | Advancing the Electrochemistry of Gasâ€Involved Reactions through Theoretical Calculations and Simulations from Microscopic to Macroscopic. Advanced Functional Materials, 2022, 32, . | 7.8 | 29 |

| # | Article | IF | Citations |
|---|---|---|---|
| 928 | New task-specific ionic liquids based on phenyl diazenyl methyl pyridinium cation: Energetic, electronic and optical properties exploration based on DFT calculations. Journal of Molecular Graphics and Modelling, 2023, 118, 108352. | 1.3 | 2 |
| 929 | Eu@C<sub>88</sub> Isomers: Calculated Relative Populations. ECS Journal of Solid State Science and Technology, 2022, 11, 101008. | 0.9 | 1 |
| 930 | Reaction Mechanisms for Chiral Phosphate Catalyzed Transformations Involving Cationic Intermediates and Protic Nucleophiles. Synlett, 0, , . | 1.0 | 0 |
| 931 | Theoretical Predictions of Fullerene Stabilities. , 2021, , 1-70. | | 0 |
| 932 | Solubility enhancement and intermolecular interactions of salicylic acid in aqueous solutions of choline chloride based deep eutectic solvents. Journal of Molecular Liquids, 2022, 367, 120433. | 2.3 | 7 |
| 933 | Assessment of advanced xDH@B3LYP methods in describing various potential energy curves driven by Ï€-Ï€, CH/Ï€, and SH/Ï€ non-bonded interactions. Chinese Journal of Chemical Physics, 2022, 35, 720-726. | 0.6 | 2 |
| 934 | Towards pharmaceutical protein stabilization: DFT and statistical learning studies on non-enzymatic peptide hydrolysis degradation mechanisms. Computational and Theoretical Chemistry, 2022, 1218, 113938. | 1.1 | 1 |
| 935 | Cluster Amplitudes and Their Interplay with Selfâ€Consistency in Density Functional Methods. ChemPhysChem, 0, , . | 1.0 | 1 |
| 936 | Towards predictive computational catalysis â€“ a case study of olefin metathesis with Mo imido alkylidene N-heterocyclic carbene catalysts. Chemical Modelling, 2022, , 1-23. | 0.2 | 1 |
| 937 | The vertical excitation energies and a lifetime of the two lowest singlet excited states of the conjugated polyenes from <scp>C2</scp> to <scp>C22</scp>: Ab initio, <scp>DFT,</scp> and semiclassical <scp>MNDOâ€MD</scp> simulations. Journal of Computational Chemistry, 2023, 44, 777-787. | 1.5 | 4 |
| 938 | Benzo[1,4]diazocinone/Pyrrole Ensembles via the Catalystâ€Free Insertion of Pyrrolylacetylenic Ketones into Benzimidazoles. ChemistrySelect, 2022, 7, . | 0.7 | 3 |
| 939 | Structure and Spectroscopic Signatures of Interstellar Sodium Isocyanate Isomers. Astrophysical Journal, 2022, 941, 40. | 1.6 | 2 |
| 940 | Quantitative Descriptions of Dewarâ€Chattâ€Duncanson Bonding Model: A Case Study of Zeise and Its Family Ions. ChemPhysChem, 2023, 24, . | 1.0 | 3 |
| 941 | Iodineâ€Catalyzed Claisenâ€Rearrangements of Allyl Aryl Ethers and Subsequent Iodocyclizations. Chemistry - an Asian Journal, 2023, 18, . | 1.7 | 6 |
| 942 | Inversion Theory Leveling as a New Methodological Approach to Antioxidant Thermodynamics: A Case Study on Phenol. Antioxidants, 2023, 12, 282. | 2.2 | 0 |
| 943 | Experimental FTIR-MI and Theoretical Studies of Isocyanic Acid Aggregates. Molecules, 2023, 28, 1430. | 1.7 | 0 |
| 944 | Theoretical study of the excitation of proflavine H-dimers in an aqueous solution: the effect of functionals and dispersion corrections. Physical Chemistry Chemical Physics, 2023, 25, 12259-12276. | 1.3 | 4 |
| 945 | Preferred intermolecular cationÂ·Â·Â·anion interactions within the [EMIM][DCA] ionic liquid and its interaction with a water co-solvent molecule. Journal of Molecular Liquids, 2023, 381, 121804. | 2.3 | 0 |

| # | Article | IF | Citations |
|---|---|---|---|
| 946 | Enhanced TSG stability through co-assembly with C3G: the mechanism behind processing Polygonum multiflorum Thunb with black beans via supramolecular analysis. Food and Function, 2023, 14, 4204-4212. | 2.1 | 2 |
| 947 | Potential Energy Surfaces Sampled in Cremerâ€“Pople Coordinates and Represented by Common Force Field Functionals for Small Cyclic Molecules. Journal of Physical Chemistry A, 2023, 127, 2646-2663. | 1.1 | 0 |
| 948 | H2OÂ·HF@C70: Encapsulation Energetics and Thermodynamics. Inorganics, 2023, 11, 123. | 1.2 | 0 |
| 949 | Complexes of a model trimeric acylphloroglucinol with a Cu<sup>2+</sup> ion: a DFT study. ChemistrySelect, 2023, . | 0.7 | 0 |
| 950 | Supramolecular Gelâ€toâ€Gel Transition Induced by Nanoscale Structural Perturbation via the Rotary Motion of Feringa's Motor. Small, 2023, 19, . | 5.2 | 3 |
| 951 | Experimental and Theoretical Study on Crown Ether-Appended-Fe(III) Porphyrin Complexes and Catalytic Oxidation Cyclohexene with O2. Molecules, 2023, 28, 3452. | 1.7 | 0 |
| 954 | Electron-density-based analysis and electron density functional theory (DFT) methods. , 2023, , 177-197. | | 0 |
| 956 | Benchmarking Modern Density Functionals for Broad Applications in Chemistry. , 2024, , 78-93. | | 0 |
| 962 | Review of Approximations for the Exchange-Correlation Energy in Density-Functional Theory. , 2023, , 1-90. | | 3 |
| 970 | Non-empirical quadratic-integrand double-hybrid (QIDH) functionals. Annual Reports in Computational Chemistry, 2023, , 87-119. | 0.9 | 0 |